Convergence of Schwarz Waveform Relaxation Methods for Systems of Semi-Linear Reaction-Diffusion Equations

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Motivation and challenges

Motivation and Issues

Reaction-Diffusion (RD) systems have extensive applications in several areas

Examples

- SEIRD models: used for modelling the spread of diseases (such as COVID-19!)
- Lotka-Volterra equations: used to model predator-prey systems

...plus other examples in mathematical biology or physics!

Finding methods to efficiently solve these systems is vital.
However, they are nonlinear, time-dependent !

Semi-linear reaction-diffusion equations

We consider, on the bounded domain $\Omega \subset \mathbb{R}^n$, the system of semi-linear RD equations

$$\begin{aligned} \partial_t \mathbf{u} - \Delta \mathbf{u} + \mathbf{f}(\mathbf{u}) &= 0 && \text{in } \Omega \times (0,T), \\ \mathbf{u}(x,t) &= \mathbf{g}(x,t) && \text{on } \partial\Omega \times (0,T), \\ \mathbf{u}(x,0) &= \mathbf{u}_0(x) && \text{in } \Omega, \end{aligned} \tag{1}$$

where $\mathbf{u} = (u_1, u_2, ..., u_d)$ and $\mathbf{f}(\mathbf{u}) = (f_1(\mathbf{u}), f_2(\mathbf{u}), ..., f_d(\mathbf{u}))$.

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where $\mathbf{u} = (u_1, u_2, ..., u_d)$ and $\mathbf{f}(\mathbf{u}) = (f_1(\mathbf{u}), f_2(\mathbf{u}), ..., f_d(\mathbf{u}))$.

Assuming that there exists a constant C such that for all $\mathbf{x}$ in $\mathbb{R}^n$, $\mathbf{f}$ satisfies

$$\|\mathbf{f}\| \leq C(1 + \|\mathbf{x}\|)$$

and under some assumptions on $\mathbf{g}$ and $\mathbf{u}_0$, the system is well-posed (Cf. Henry '81)

Motivation of this work

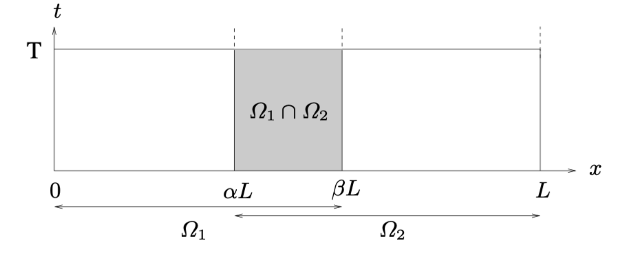
Study and develop Schwarz waveform relaxation (SWR) methods the their optimised versions for non-linear systems of PDEs

- convergence study when applied to semi-linear RD systems.
- show superlinear convergence on bounded time intervals and linear (under conditions) over long time by using comparison principles.
- derive optimised versions on the linear counterpart and apply them to nonlinear systems.

SWR Methods

What are Schwarz waveform relaxation (SWR) methods?

- SWR are a type of domain decomposition method - the overall domain is divided into smaller **sub-domains** on which the system is solved.
- they rely on a space-time decomposition with **overlapping** sub-domains.



Decompose the domain into overlapping sub-domains $\Omega_1 = (0, \beta L)$ and $\Omega_2 = (\alpha L, L)$, $\alpha < \beta$.

Denoting $\mathbf{g_1}(t) := \mathbf{g}(0,t)$ and $\mathbf{g_2}(t) := \mathbf{g}(L,t)$, the SWR method gives at iteration $n+1$ the approximate solutions $\mathbf{v}^{n+1}$, $\mathbf{w}^{n+1}$ on the two sub-domains by solving the equations

$$\begin{array}{rcll} \partial_t \mathbf{v}^{n+1} - \Delta \mathbf{v}^{n+1} + \mathbf{f}(\mathbf{v}^{n+1}) & = & 0 & \text{in } \Omega_1 \times (0,T), \\ \mathbf{v}^{n+1}(0,t) & = & \mathbf{g}_1(t) & \text{on } (0,T), \\ \mathbf{v}^{n+1}(\beta L, t) & = & \mathbf{w}^n(\beta L, t) & \text{on } (0,T), \\ \mathbf{v}^{n+1}(x,0) & = & \mathbf{u}_0(x) & \text{in } \Omega_1 \end{array} \tag{2}$$

$$\begin{array}{rcll} \partial_t \mathbf{w}^{n+1} - \Delta \mathbf{w}^{n+1} + \mathbf{f}(\mathbf{w}^{n+1}) & = & 0 & \text{in } \Omega_2 \times (0,T), \\ \mathbf{w}^{n+1}(\alpha L,t) & = & \mathbf{v}^n(\alpha L,t) & \text{on } (0,T), \\ \mathbf{w}^{n+1}(L, t) & = & \mathbf{g}_2(t) & \text{on } (0,T), \\ \mathbf{w}^{n+1}(x,0) & = & \mathbf{u}_0(x) & \text{in } \Omega_2. \end{array} \tag{3}$$

We denote the errors in sub-domain Ω_1 by $\mathbf{d}^n := \mathbf{u} - \mathbf{v}^n$ and in Ω_2 by $\mathbf{e}^n := \mathbf{u} - \mathbf{w}^n$.

Linear Convergence Estimate

Assume that $\partial_i f_i \geq 0$, $i = 1, ..., d$, and that there exists a constant a satisfying $0 < a < (\pi/L)^2$, such that $-\frac{a}{d} \leq \partial_i f_j \leq 0$, $j \neq i$. Then the errors in the Schwarz waveform relaxation algorithm satisfy

$$\sup_{x\in\Omega_1} \|\mathbf{d}^{2n+1}(x,\cdot)\|_\infty \leq \gamma^n \|\mathbf{e}^0(\beta L,\cdot)\|_\infty, \tag{4}$$

$$\sup_{x\in\Omega_2} \|\mathbf{e}^{2n+1}(x,\cdot)\|_\infty \leq \gamma^n \|\mathbf{d}^0(\alpha L,\cdot)\|_\infty, \tag{5}$$

where $\gamma \in (0,1)$ is given by

$$\gamma = \left(\frac{\sin(\sqrt{a}\alpha L)}{\sin(\sqrt{a}\beta L)}\right)\left(\frac{\sin(\sqrt{a}(1-\beta)L)}{\sin(\sqrt{a}(1-\alpha)L)}\right).$$

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Superlinear Convergence Estimate

Under same assumption on application f, the errors in the Schwarz waveform relaxation algorithm satisfy

$$\sup_{x\in\Omega_1} \|\mathbf{d}^{2n}(x,\cdot)\|_T \leq \max(e^{aT},1)\text{erfc}\left(\frac{n(\beta-\alpha)L}{\sqrt{T}}\right)\|\mathbf{d}^0(\beta L,\cdot)\|_T, \quad (6)$$

$$\sup_{x\in\Omega_2} \|\mathbf{e}^{2n}(x,\cdot)\|_T \leq \max(e^{aT},1)\text{erfc}\left(\frac{n(\beta-\alpha)L}{\sqrt{T}}\right)\|\mathbf{e}^0(\alpha L,\cdot)\|_T, \quad (7)$$

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Let $T > 0$ and let $\mathbf{u} = (u_j)_{1 \leq j \leq d} \in C^{2,1}(\Omega \times [0,T))^d$ be a function for which each component satisfies

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\begin{aligned}
\partial_t u_i - \Delta u_i + \sum_{j=1}^{d} a_{ij}(x,t) u_j &= 0, \quad \text{in } \Omega \times (0,T) \\
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Let $\tilde{a}$ be a constant and $\tilde{u} \in C^{2,1}(\Omega \times [0,T))$ be a scalar function satisfying

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We assume that $A(x,t) = (a_{ij}(x,t))_{1\le i,j\le d}$ verifies

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and that for $i = 1, ..., d$ and for all $t \in [0,T]$,

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Then for $i = 1, ..., d$,
$|u_i(x,t)| \le \tilde{u}(x,t)$, $\forall (x,t) \in \Omega_T = \Omega \times (0,T]$.

Numerical results

The model:

$$\begin{cases} \partial_t u - \nu_u \Delta u - u(1 - u - rv) = 0, \\ \partial_t v - \nu_v \Delta v - buv = 0 \end{cases}$$

with $(b, r > 0)$ example of non-equilibrium thermodynamics, resulting in the establishment of a nonlinear chemical oscillator.

- the main aspect of the reaction is its 'excitability'
- the ratio of concentration of some ions oscillated, causing the colour of the solution to change.

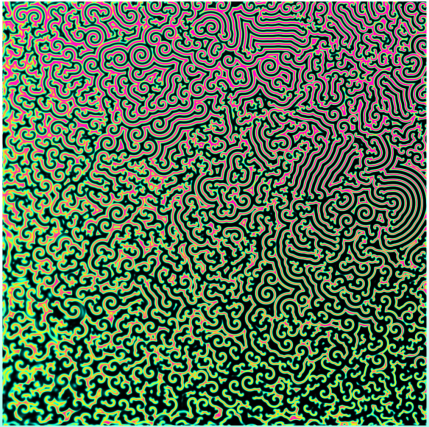

Figure 1: Credits: Wikimedia Commons

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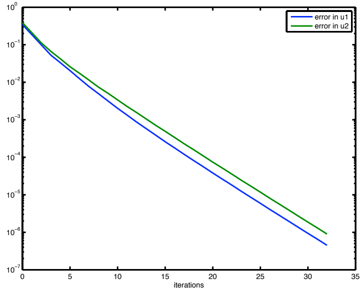

Figure 1: Variable change $\bar{u} = 1 - u \Rightarrow$ the hypothesis of the Theorem are verified $\Rightarrow$ linear convergence.

FitzHugh-Nagumo equations

The model:

$$\begin{cases} \partial_t u - \nu_u \Delta u - f(u) + \sigma v = 0, \\ \partial_t v - \nu_v \Delta v - u + v = 0 \end{cases}$$

with $f(u) = \lambda u - u^3 - \kappa$ $(\lambda, \nu_u, \nu_v, \kappa > 0)$ describes how an action potential travels through a nerve.

- prototype of an excitable system (e.g., a neuron).
- activator-inhibitor type of system: close to the ground state, one component stimulates the production of both components while the other one inhibits their growth.

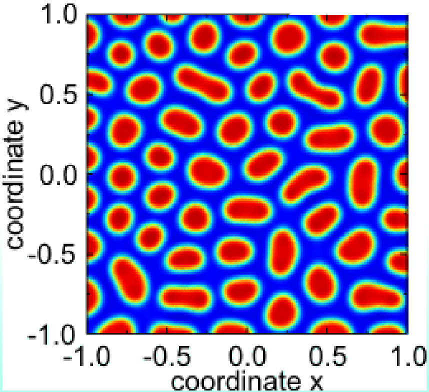

Figure 2: Credits: Wikipedia

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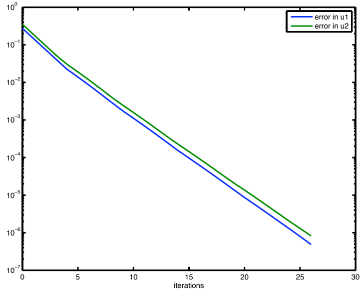

Figure 2: The hypothesis of the Theorem are not verified BUT we still have linear convergence.

The model (with migration of the populations):

$$\begin{cases} \partial_t u - \nu_u \Delta u - u(\alpha - \beta v) = 0, \\ \partial_t v - \nu_v \Delta v + v(\gamma - \delta u) = 0 \end{cases}$$

describe a biological system in which two species interact, one a predator and one its prey.

- prey population is assumed to have an unlimited food supply, and to reproduce exponentially unless subject to predation
- predator population grows fueled by the food supply, minus natural death.

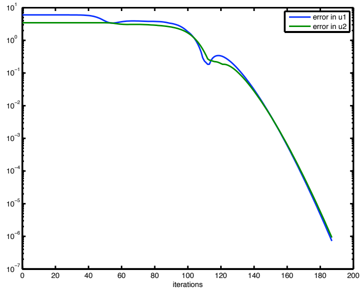

Figure 3: The hypothesis of the Theorem are not verified, we have convergence but not the linear one.

Optimised SWR (OSWR) Methods

Optimised Method: Introduction

Idea: (from Y. Courvoisier thesis, University of Geneva) optimise the method for a nearby linear system and see how it works for non-linear system. Consider RD systems of the form

$$\partial_t \mathbf{u} = D\partial_{xx}\mathbf{u} - B\mathbf{u},\ \mathbf{u} = (u, v),$$

where D and B are constant in space matrices in $\mathbb{R}^{2\times 2}$ such that the matrix D is positive definite and the eigenvalues of B are positive.

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Further assumption: D and B can be diagonalised in the same basis, allowing us to diagonalise our system. This leads to the uncoupled system

$$\begin{cases} \tilde{u}_t = \nu_1 \tilde{u}_{xx} - \lambda_1 \tilde{u}, \\ \tilde{v}_t = \nu_2 \tilde{v}_{xx} - \lambda_2 \tilde{v}. \end{cases}$$

We can now focus on a single equation when obtaining our optimisation.

Simplified Equation and Method

Focus on the one-dimensional linear RD equation:

$$u_t = \nu u_{xx} - \lambda u, \ \nu, \lambda > 0,$$

with initial condition $u(x, 0) = g(x)$.

Simplified Equation and Method

Focus on the one-dimensional linear RD equation:

$$u_t = \nu u_{xx} - \lambda u, \;\; \nu, \lambda > 0,$$

with initial condition $u(x,0) = g(x)$. SWR algorithm with Robin transmission conditions gives

$$\begin{cases} \partial_t u_1^n = \nu \partial_{xx} u_1^n - \lambda u_1^n, & \Omega_1 \times (0, \infty) \\ (\partial_{\mathbf{n}_1} + p) u_1^n = (\partial_{\mathbf{n}_1} + p) u_2^{n-1}, & \partial\Omega_1 \times (0, \infty) \\ u_1^n(x, 0) = g(x), & \Omega_1 \end{cases}$$

$$\begin{cases} \partial_t u_2^n = \nu \partial_{xx} u_2^n - \lambda u_2^n, & \Omega_2 \times (0, \infty) \\ (\partial_{\mathbf{n}_2} + p) u_2^n = (\partial_{\mathbf{n}_2} + p) u_1^{n-1}, & \partial\Omega_2 \times (0, \infty) \\ u_2^n(x, 0) = g(x), & \Omega_2, \end{cases}$$

where $\mathbf{n}_1$ and $\mathbf{n}_2$ are the unit outward vectors of Ω_1 and Ω_2 respectively, and p is the Robin parameter.

Computation of the contraction Factor

Fourier transform in time + computation of the local errors + iterate ⇒ contraction factor for our SWR algorithm:

$$\rho(\omega, \lambda, \nu, p) = \left| \left(\frac{p - \sqrt{\alpha}}{p + \sqrt{\alpha}} \right)^2 e^{-2\sqrt{\alpha} L} \right|, \ \alpha := \frac{i\omega + \lambda}{\nu}$$

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Rewrite $\alpha = \frac{i\omega+\lambda}{\nu}$ in the form $\alpha = i\tilde{\omega} + \frac{\lambda}{\nu}$, where $\tilde{\omega} = \frac{\omega}{\nu}$.

$$f(p, y) = \frac{(p - y)^2 + y^2 - \varepsilon}{(p + y)^2 + y^2 - \varepsilon} e^{-2yL}, \; \varepsilon = \frac{\lambda}{\nu}$$

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A lot of different cases + tedious computations + different cases to be considered...but the optimal parameter can be found!

Numerical Results - OSWR

Discretising the OSWR method

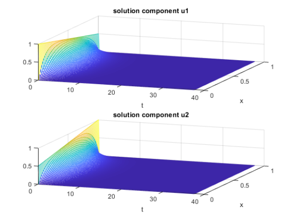
Discretise (implicit Euler for the linear part and explicit for the nonlinear part)

$$\boldsymbol{u}_t = \nu \boldsymbol{u}_{xx} - \boldsymbol{f}(\boldsymbol{u}), \;\; \boldsymbol{u} = [u,\, v]^T$$

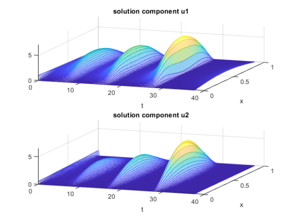
For our implementation, set the following values: $[a, b] = [0, 1]$, $[0, T] = [0, 12\pi]$, $\nu = 0.05$, $N = 60$ and $M = 200$. Initial condition $\boldsymbol{u}_0 = [1 - x/2, 1/2 + x/2]^T$ and boundary conditions $\boldsymbol{u}_a = \boldsymbol{u}_b = \boldsymbol{0}$.

Linear Example: $\boldsymbol{f}(\boldsymbol{u}) = \lambda \boldsymbol{u}$ and $\nu = 0.05$ and $\lambda = 0.05$.

Non-Linear Example: $\boldsymbol{f}(\boldsymbol{u}) = [u - uv, -u + uv]^T$.



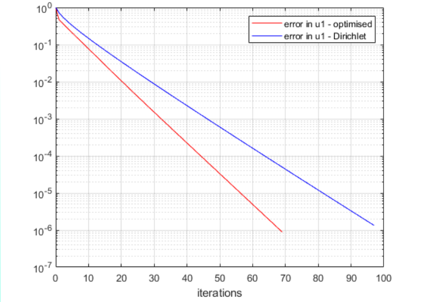
Computed solution for linear example

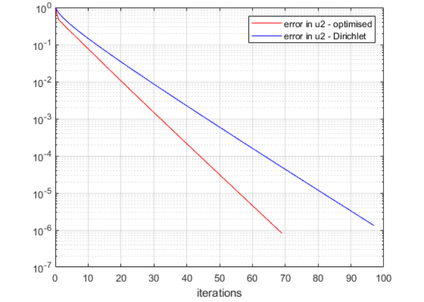


Computed solution for non-linear example

Linear Example, small overlap

- We run the algorithm for values in the interval $p = [0.1, \sqrt{\varepsilon}]$.
- Robin algorithm outperforms Dirichlet even when p is sub-optimal.
- Best rate of convergence obtained for $p = \sqrt{\varepsilon}$, in accordance with theory.





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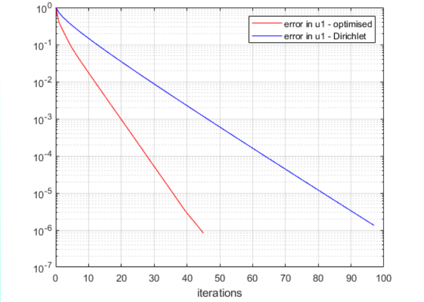

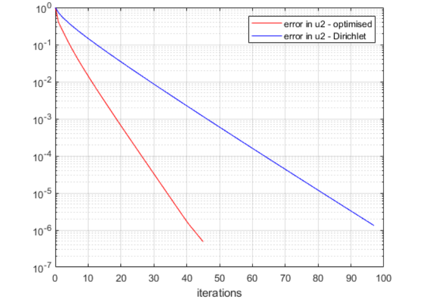

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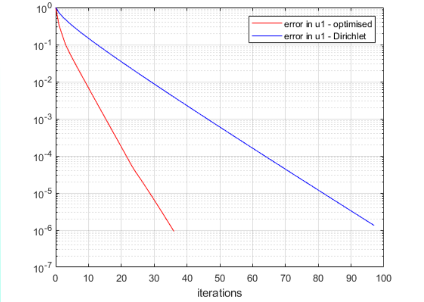

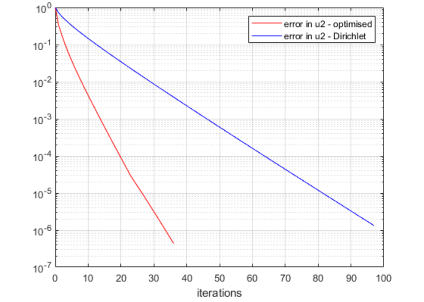

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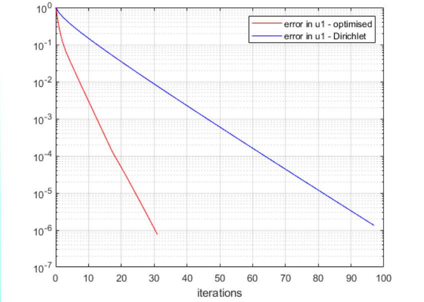

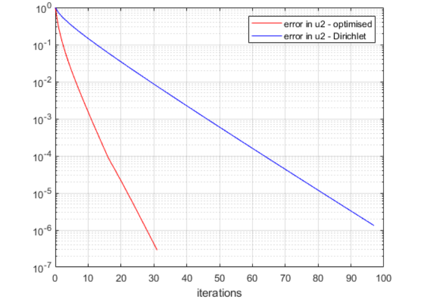

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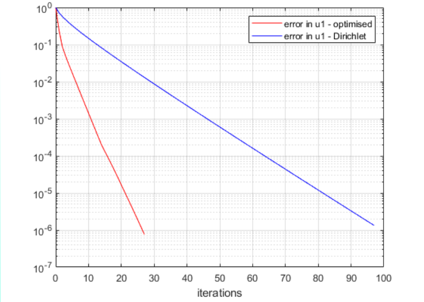

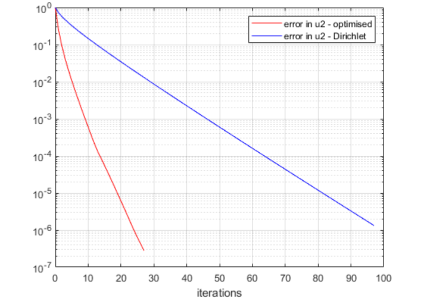

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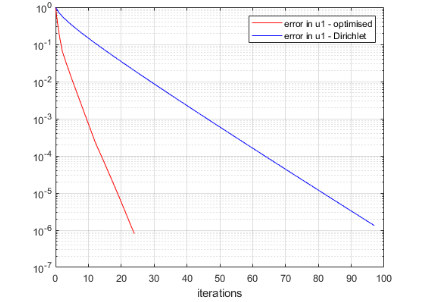

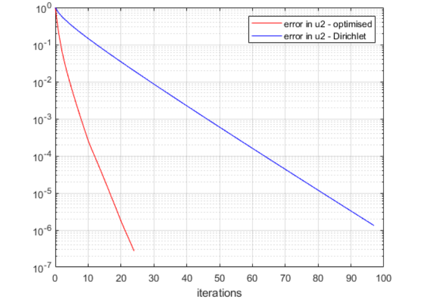

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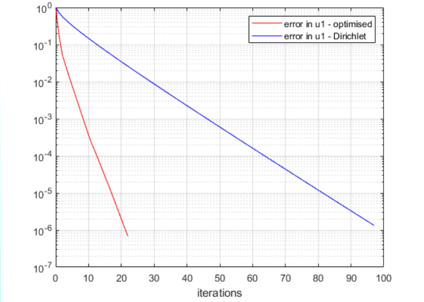

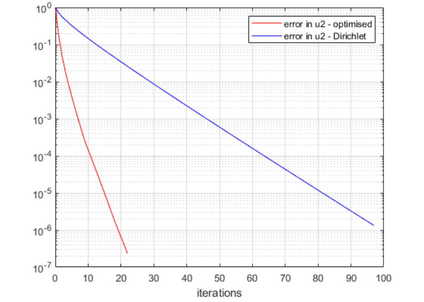

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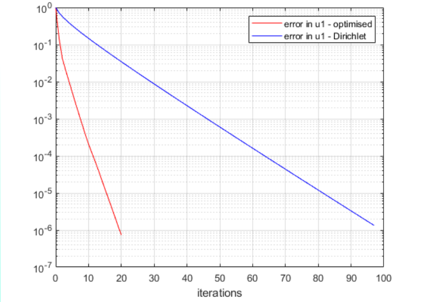

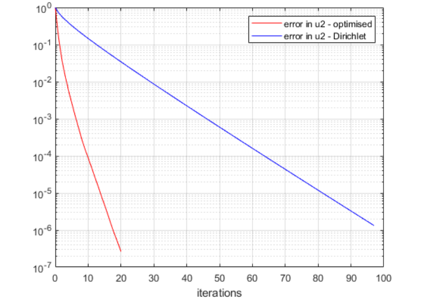

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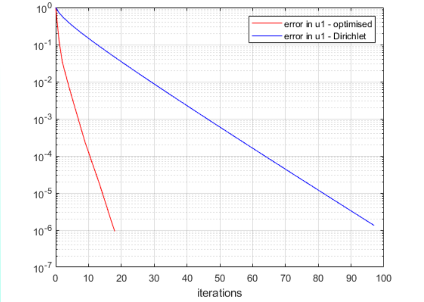

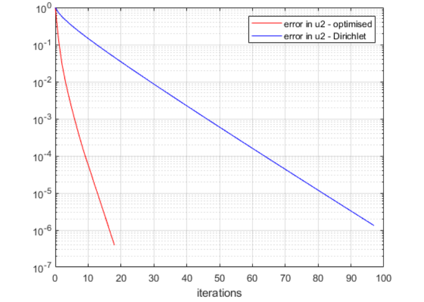

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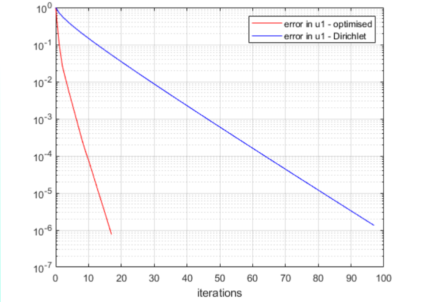
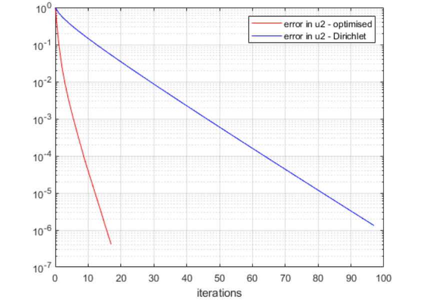
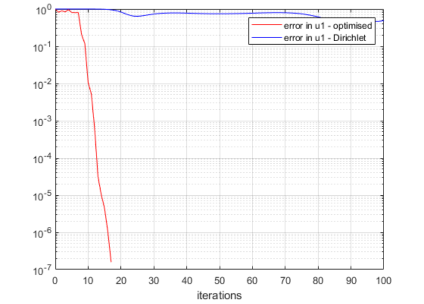
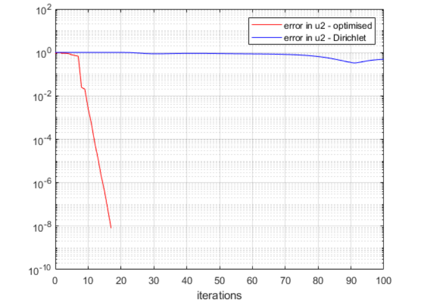




Non-Linear Example: small vs large overlap

- We vary the value of p from 1 to 10, with small then large overlap.
- Dirichlet fails to converge - optimised method successfully converges for $p \geq 4$.
- Best rate of convergence obtained for $p = 4$. (not in line with the theoretical results)





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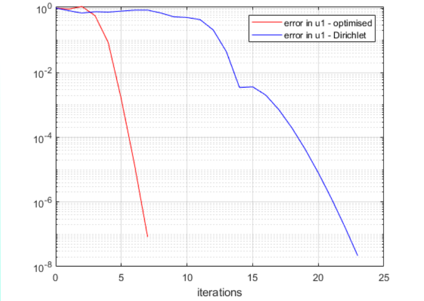
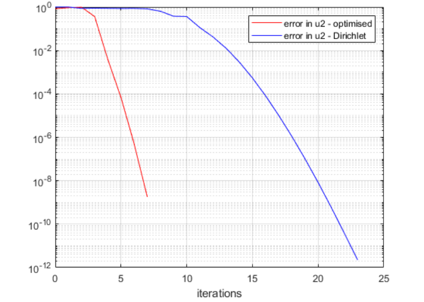
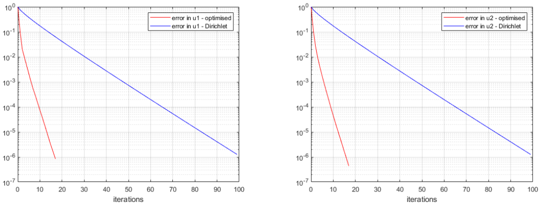


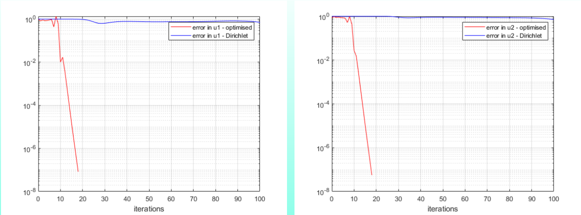


Altered Boundary Conditions



Error plot: Linear Example, $p = 1$.

- OSWR remains superior over SWR
- Optimal value of p occurs at $p = 1$; unchanged from original boundary conditions



Error plot: Non-Linear Example, $p = 4$.

- OSWR converges rapidly even when SWR fails to converge
- Optimal value of p occurs at $p = 4$; unchanged from original boundary conditions

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- Theoretical convergence analysis for SWR applied to semi-linear RD system.
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However, it is clear further research could be done into the efficiency of this method.

Further Research Examples

- Investigate the limitation on the value of the Robin parameter p.
- Test the method on a more complex non-linear systems, such as an SEIRD model.
- Research the effectiveness of the method for higher dimensional systems.