Overview of Schwarz waveform relaxation domain decomposition methods for the Schrödinger equation

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Outline

Goal: Derivation & analysis of SWR domain decomposition methods for linear & nonlinear quantum wave equation

Outline

Schwarz Waveform Relaxation (SWR) Algorithm

SWR: *iterative* meth. for solving in parallel (evol.) PDE

- Extensively used... but math. analysis still incomplete...
- We study Schrödinger $P = \mathrm{i}\partial_t + \triangle - V(\mathbf{x})$ (space dep. pot.)
- ...in imaginary (stationary) & real time (evolution)
- + discussion for nonlinear case: $+\kappa|\phi|^2\phi$

We prop. "general" approac. [for all types of wave eq.]

- **analysis** *convergence rate* / **transmission conditions**
- ... using pseudodiff. calc. & symbolic asympt. expansions

References

[A. Quarteroni, A. Valli, DDM for PDE, Oxford Publi., '99], [V. Dolean, P. Jolivet, F. Nataf, SIAM '15],
[M. Gander's papers, '00-'17], [F. Nataf, F. Nier, CPDE'98(23)], [L. Halpern, F. Nataf, SINUM'03 (41)]

Schwarz Waveform Relaxation Algorithm (1-d)

Start with IVP (wave, Schrödinger, Klein-Gordon,... denoted P)

$$P\phi(x,t) = 0,\ x \in \mathbb{R},\ t > 0, \qquad \phi(x,0) = \phi_0(x),\ x \in \mathbb{R}$$

Two-domains $\mathbb{R} = \Omega_\varepsilon^+ \cup \Omega_\varepsilon^-$

- $\Omega_\varepsilon^+ = \big(-\infty, +\varepsilon/2\big)$, $\Omega_\varepsilon^- = \big(-\varepsilon/2, +\infty\big)$, $\quad \varepsilon \geqslant 0$
- overlap: $\Omega_\varepsilon^+ \cap \Omega_\varepsilon^- = (-\varepsilon/2, +\varepsilon/2)$
- $\phi^\pm$ solution in $\Omega_\varepsilon^\pm$

$$\left\{\begin{array}{lcll} P\phi^\pm & = & 0, & x \in \Omega_\varepsilon^\pm,\ t > 0, \\ \phi^\pm(\cdot,0) & = & \phi_{0|\Omega_\varepsilon^\pm}, & x \in \Omega_\varepsilon^\pm, \\ B^\pm\phi^\pm\big(\pm\varepsilon/2,\cdot\big) & = & B^\pm\phi^\mp\big(\pm\varepsilon/2,\cdot\big), & t > 0 \end{array}\right.$$

- $B^\pm$ operator TBD...
- Systems are *coupled* through BC... no parallelism...
- No guarantee that $\phi^\pm = \phi_{|\Omega_\varepsilon^\pm}$

Schwarz Waveform Relaxation Algorithm (1-d)

Schwarz Waveform Relaxation

- *Iterative* process allows for...
- ....decoupling of 2 systems in $\Omega_\varepsilon^\pm$

At *Schwarz iteration* $k \geqslant 1$

$$
\left\{
\begin{array}{rcll}
P\phi^{\pm,(k)} & = & 0, & x \in \Omega_\varepsilon^\pm,\ t > 0, \\
\phi^{\pm,(k)}(\cdot, 0) & = & \phi_{0|\Omega_\varepsilon^\pm}, & x \in \Omega_\varepsilon^\pm, \\
B^\pm\phi^{\pm,(k)}\big(\pm\varepsilon/2, \cdot\big) & = & B^\pm\phi^{\mp,(k-1)}\big(\pm\varepsilon/2, \cdot\big), & t > 0
\end{array}
\right.
$$

- $\phi^{\pm,(k=0)}\big(\mp\varepsilon/2, \cdot\big)$ are two given functions
- $B^\pm$ *transmission* operator TBD...
- *Schwarz Iter.* $=$ *price for uncoupled (decomp.) syst. (dom.)*

Schwarz Waveform Relaxation Algorithm (1-d)

Expect subdom. sol $\phi^{\pm}$ conv. (in appropriate space) to $\phi_{|\Omega_{\varepsilon}^{\pm}}$

$$\phi^{\pm,(k)} \to_{k\to+\infty} \phi_{|\Omega_{\varepsilon}^{\pm}}$$

In practice: k_0 iterations. How to select $B^{\pm}$ for k_0 small ?

- If $B^{\pm} = Id$: Dirichlet-based T.C. *Classical* SWR (CSWR):

$$\phi^{\pm,(k)}\big(\pm\varepsilon/2,\cdot\big) \quad = \quad \phi^{\mp,(k-1)}\big(\pm\varepsilon/2,\cdot\big)$$

  In general slow convergence: k_0 *large*, $\varepsilon > 0$....

- Fast convergence: *(k_0 small)*. Design $B^{\pm}$ from Transparent/Absorbing BC for wave eqs (!)

Use *technology* developed for TBC/ABC

Derivation - TBC/ABC: Nirenberg Factorization

Say op. P (ex: Schrö.) factorization at boundary

$$P = \big(\partial_x + \mathrm{i}\Lambda^-\big)\big(\partial_x + \mathrm{i}\Lambda^+\big) + R \qquad \big(R \in OPS^{-\infty} := \cap_m OPS^m\big)$$

where at interface (in hyperb. zone)

- $\partial_x + \mathrm{i}\Lambda^-$: op. corresponding incoming wave
- $\partial_x + \mathrm{i}\Lambda^+$: op. corresponding outgoing wave
- Ex. $\mathrm{i}\Lambda^\pm = \pm\partial_t$ (wave), $\mathrm{i}\Lambda^\pm = \pm e^{-\mathrm{i}\pi/4}\sqrt{\partial_t}$ (Schrö. $V = 0$)

To AVOID/REDUCE reflection (TBC/ABC)... impose

$$\big(\partial_x + \mathrm{i}\Lambda^+\big)\phi = 0 \text{ at boundary \& any time}$$

$\Lambda^\pm$ computed explicitly(!) using pseudodiff. calc. [L. Nirenberg, AMS'73],[L. Hörmander, Springer'76],[A. Majda, B. Engquist '77]

- $\Lambda^\pm = \sum_{j\geqslant 0} \Lambda^\pm_{1/2-j/2}$. Series of decreas. order pseudodiff. op.
- $\Lambda^\pm \approx \Lambda^\pm_M := \sum_{0\leqslant j\leqslant M} \Lambda^\pm_{1/2-j/2}$ (coinc. up to order $-M/2$ op.)

Factorization (microlocal analysis)

Search *classical symbols* Λ^+ as in [X. Antoine, C. Besse, '03], $t \leftrightarrow \tau$ (dual)

Plug $\sigma_t(\Lambda^+) = \lambda^+(x,\tau) \sim \sum_{j\geqslant 0} \lambda^+_{1/2-j/2}(x,\tau)$ in

$$\Big(\partial_x + \mathrm{i}\sum_{j\geqslant 0}\lambda^-_{1/2-j/2}(x,\tau)\Big)\Big(\partial_x + \mathrm{i}\sum_{j\geqslant 0}\lambda^+_{1/2-j/2}(x,\tau)\Big)$$

and identify with symbol $\sigma_t(P)$ of P

- Λ^+ approx. by $\Lambda^+_M := Op(\sum_{0\leqslant j\leqslant M}\lambda^+_{1/2-j/2})$ with
- $\Lambda^+ \approx \Lambda^+_M$ up to op. of order $-M/2$. If $|\tau|$ large, take M small
- $\Lambda^\pm$ (outgoing/incoming rays) : via *Null bicharact. strips* at in *hyperb. reg. of cotang. bundle at bound.* $T^*(\partial\Omega \times [0,T])$.

Zoology of transmission operators for SWR

Once $\Lambda^{\pm}$ constructed: Transmission Op. $B^{\pm}$

- $B^{\pm} = \mathrm{I}$: *Classical* SWR (Dirichlet T.C.)
- $B^{\pm} = \partial_x + \mathrm{i}\Lambda^{\pm}$: *Optimal* SWR (*nonlocal* transparent T.C.)
- $B^{\pm} = \partial_x + \mathrm{i}\Lambda^{\pm}_M$: *Mth-Optimal* SWR (*non-local* absorbing T.C.)
- $B^{\pm} = \partial_x + \mathrm{i}\lambda^{\pm}_{\mathrm{Opt}}$: *Optimized* SWR (Robin with opt. const.)
  ... also $B^{\pm} = \partial_x + \mathrm{i}\Lambda^{\pm}_{M=0}$
- $B^{\pm} = \partial_x + \mathrm{i}P^{\pm}_M(x,t)$ *Lagrange* SWR (*local* T.C.):

$$P^{\pm}_M = \mathrm{Op}(p^{\pm}_M), \qquad \text{with } p^{\pm}_M\text{-d}^{o}M \text{ Lagrange poly. of } \sigma(\Lambda^{\pm}_M)$$

SWR method performance

Summary: rate of convergence is $B^{\pm}$-dependent

Trans.Cond.	Converg. rate	Comput. complex.	Memory
Optimal (Transp.)	☺ ☺	☹ ☹	☹ ☹
Optimized (Robin)	☺	☺ ☺	☺ ☺
Classical (Diri.)	☹	☺ ☺	☺ ☺
Lagrange	☺ ☺	☺	☺

Compromise : conv. rate / comput. complex. / memo. usage

Some analytical details and experiments...

Optimal Schwarz Waveform Relaxation Algorithm

From $\Lambda^{\pm}$: Optimal Schwarz RW, at iteration $k \geqslant 1$

$$
\begin{cases}
P\phi^{\pm,(k)} = 0, & x \in \Omega_{\varepsilon}^{\pm},\ t > 0, \\
\phi^{\pm,(k)}(\cdot, 0) = \phi_0^{\pm}, & x \in \Omega_{\varepsilon}^{\pm}, \\
(\partial_x + \mathrm{i}\Lambda^{\pm})\phi^{\pm,(k)}\big(\pm\varepsilon/2, \cdot\big) = (\partial_x + \mathrm{i}\Lambda^{\pm})\phi^{\mp,(k-1)}\big(\pm\varepsilon/2, \cdot\big)
\end{cases}
$$

where

- exact OSWR: $\Lambda^{\pm}$ / $P = (\partial_x + \mathrm{i}\Lambda^{+})(\partial_x + \mathrm{i}\Lambda^{-})$
- in practice: Mth-OSWR take $\Lambda^{\pm} \approx \Lambda_M^{+} := \sum_{0 \leqslant j \leqslant M} \Lambda_{1/2-j/2}^{+}$

Fast CV in *real time* LSE [L. Halpern, J. Szeftel, M3AS'10],[X. Antoine, E. Lorin, J. Sc. Comput.'15]

SWR Schrödinger in real-time: well-posed. & convergence I

Theorem (well-posedness)

Let $\varepsilon > 0$, $V \in L^\infty(\Omega_\varepsilon^- \cup \Omega_\varepsilon^+)$. CSWR defines iterates $(\phi^{+,(k)}, \phi^{-,(k)})$ in $H^{2,1}(\Omega_{\varepsilon/2}^+ \times (0,T)) \times H^{2,1}(\Omega_\varepsilon^- \times (0,T))$ with $\phi^{+,(k)}(-\varepsilon/2,\cdot)$, $\partial_x\phi^{+,(k)}(-\varepsilon/2,\cdot)$, $\phi^{-,(k)}(\varepsilon/2,\cdot)$ and $\partial_x\phi^{-,(k)}(\varepsilon/2,\cdot)$ in $H^1(0,T)$.

Theorem (convergence)

For $(h^-,h^+) \in (H^{3/4}(0,T))^2$ with $h^-(0) = \phi_0(-\varepsilon/2)$ and $h^+(0) = \phi_0(\varepsilon/2)$. Let V be a real constant, $\tau_{max} > 0$ such that $(e^{-t}h^\pm)$ vanishes outside $[-\tau_{max}, +\infty)$, with $g^+ = h^+ - \phi^+(-\varepsilon/2,\cdot)$ and $g^- = h^- - \phi^-(\varepsilon/2,\cdot)$. Then $(\phi^{-,(k)}, \phi^{+,(k)})$ converges in $L^2(\Omega_\varepsilon^+ \times (0,T)) \times L^2(\Omega_\varepsilon^- \times (0,T))$.

[L. Halpern, J. Szeftel, M3AS '10], [M. Gander, L. Halpern, SINUM'07] and [X. Antoine, E. Lorin, J. Comput. App. Math., '19] in 2d.

SWR Schrödinger in real-time: well-posed. & convergence II

For linear Schrödinger eq.

Theorem (Halpern-Szeftel '10)

- *For $V = 0$: Optimal SWR ($B^{\pm} = \partial_x \pm \sqrt{\mathrm{i}\partial_t}$): conv. in 2 Schwarz it. for the one-dim., even without overlap ($\varepsilon = 0$).*
- *For: $B^{\pm} = \partial_x \pm \sqrt{\mathrm{i}\partial_t + V(0)}$. For V, V' in $L^{\infty}(\mathbb{R})$. conv. proven in $H^{1/4}(0, T, L^2(\Omega_1)) \cap H^{-1/4}(0, T, H^1(\Omega_1)) \times H^{1/4}(0, T, L^2(\Omega_2)) \cap H^{-1/4}(0, T, H^1(\Omega_2))$.* **But no CV rate.**

For 1d linear advection+diffusion+react. (constant coeff.) eq.

Theorem (Gander-Halpern '07)

- *Convergence rate: CSWR $\ll$ Optimized SWR*

[L. Halpern, J. Szeftel, M3AS '10], [M. Gander, L. Halpern, SINUM'07]

Convergence CSWR algorithm in imaginary time

Convergence rate of CSWR in imaginary time

Theorem (Antoine, Lorin '17)

Imaginary time method for linear 1-d Schrödinger:

- *V smooth/bounded/spatial dependent & overlap size $\varepsilon > 0$*
- *CSWR* **conv. rate** *in X [fixed point algo. contrac. fact.]*

$$C_C^{IT} = \sup_{\tau\in\mathbb{R}} L_C^{IT}(\tau) \approx \exp\Big(-\varepsilon\sqrt{2|\tau|} - \int_{-\varepsilon/2}^{\varepsilon/2} V(y)dy/\sqrt{2|\tau|}\Big)$$

- $X = H^{3,3/2}(\Omega_\varepsilon^+ \times (0, T^{(k_{cvg})})) \times H^{3,3/2}(\Omega_\varepsilon^- \times (0, T^{(k_{cvg})}))$

Convergence rate OSWR: LSE in *imaginary time*

Convergence rate of Mth-OSWR in imaginary time

Theorem (Antoine, Lorin '17)

Assume $\Lambda^{\pm} \approx \Lambda^{\pm,M} := \sum_{j=0}^{M} \Lambda^{\pm}_{1/2-j/2}$, *and* $M \in \mathbb{N}^*$.
Conv. rate *for Mth-OSWR:* $C^{IT}_{O;M} = \sup_{\tau} L^{IT}_{O;M}(\tau)$ *where*

$$L^{O,M}_{\varepsilon}(\tau) \approx \quad \boldsymbol{c^{M}_{\varepsilon}|\tau|^{-(M+1)}} L^{C}_{\varepsilon}(\tau), \qquad \textit{for } |\tau| \textit{ large}$$

with $\lambda^{\pm}_{1/2-j/2} = \sigma\left(\Lambda^{\pm}_{1/2-j/2}\right)$ *(symbol) and* $c^{M}_{\varepsilon} \in \mathbb{R}^{*}_{+}$

- Accel. of conv. Mth-OSWR vs CSWR thanks to $1/|\tau|^{M+1}$-term
- No overlap needed ($\varepsilon = 0$) for Mth-OSWR.

Proof NLSE imaginary time

Ingredients of the proof:

- Rewrite conv. prob. as fixed point eq. on error function
- ... in (x, τ)-space
- Determine contraction factor of from Lipschitz mapping...
- ...using asymptotic expansion of symbols $\lambda^{\pm}$

Details: [X. Antoine, E. Lorin, Numerische Math., 2017].

NLSE and other extension

Extension to NLSE. No proof (needs paradiff. calc.)... but...

- Close to conv. $\kappa|\phi|^2$ behaves as linear potential $\kappa|\phi_\ell|^2$

Contraction factor estimate in asympt. regime.

$$C_{\mathrm{C}}^{\mathrm{IT}}(\tau) \approx \sup_{\tau} \exp\Big(-\varepsilon\sqrt{2|\tau|} - \frac{1}{\sqrt{2|\tau|}}\int_{-\varepsilon/2}^{\varepsilon/2}\big[V(y) + \kappa|\phi_\ell(y)|^2\big]dy\Big).$$

Pseudodiff. strategy still applicable to...

- time-dependent Schrödinger

$$\mathtt{i}\partial_t\psi(x,t) = -\triangle\,\psi(x,t) + V(x)\psi(x,t)$$

- in symbols $\lambda(x,\tau) \mapsto \lambda(x,-\mathtt{i}\tau)$... and derive CF
- other wave eqs. (Klein-Gordon, Dirac, ...) & higher dimension

Proof extended to multi-subdomain [X. Antoine, E. Lorin, Multiscale Sc. Eng., 2019].

Convergence rate

Conv. rate (for $|\tau|$ large): **Contrac. Fact.** fixed point algo.

- $C_{\mathrm{C}}^{\mathrm{IT}} \approx \sup_{\tau\in\mathbb{R}} \exp\Big(-\varepsilon\sqrt{2|\tau|} - \int_{-\varepsilon/2}^{\varepsilon/2} V(y)dy/\sqrt{2|\tau|}\Big)$
- $C_{\mathrm{O};M}^{\mathrm{IT}} =$
  $\sup_{\tau\in\mathbb{R}} \boldsymbol{c_{\varepsilon}^{M}|\tau|^{-(M+1)}} \exp\Big(-\varepsilon\sqrt{2|\tau|} - \int_{-\varepsilon/2}^{\varepsilon/2} V(y)dy/\sqrt{2|\tau|}\Big)$
- $C_{\mathrm{Opt}}^{\mathrm{IT}} = C_{\mathrm{O};M=0}^{\mathrm{IT}}$
- $C_{\mathrm{C}}^{\mathrm{RT}} = \sup_{\tau\in\mathcal{E}_{\tau}} \exp\Big(-2\varepsilon\sqrt{-\tau} + \dfrac{1}{2\sqrt{-\tau}}\int_{-\varepsilon/2}^{\varepsilon/2} V(y)dy\Big)$
- $C_{\mathrm{O};M}^{\mathrm{RT}} =$
  $\sup_{\tau\in\mathcal{E}_{\tau}} \boldsymbol{c_{\varepsilon}^{M}|\tau|^{-(M+1)}} exp\Big(-2\varepsilon\sqrt{-\tau} + \dfrac{1}{2\sqrt{-\tau}}\int_{-\varepsilon/2}^{\varepsilon/2} V(y)dy\Big)$
- $C_{\mathrm{Opt}}^{\mathrm{RT}} = C_{\mathrm{O};M=0}^{\mathrm{RT}}$

$\mathcal{E}_{\tau}$: elliptic zone of T.C.

Numerics: NLSE imaginary time

Discretization for SWR NGF/NLSE 1d: Semi-Implicit-Euler

- **Convergence criterion for NGF at Schwarz it. $k \to T^{(k)}$**

$$\|\phi^{n+1,(k)} - \phi^{n,(k)}\|_\infty \leqslant \delta,$$

- **Convergence criterion for Schwarz DDM $k^{(\mathrm{cvg})}$**

$$\Big\| \ \|\phi^{+,\mathrm{cvg},(k)}_{|\Gamma_\varepsilon} - \phi^{-,\mathrm{cvg},(k)}_{|\Gamma_\varepsilon}\|_{\infty,\Gamma_\varepsilon} \Big\|_{L^2(0,T^{(k^{\mathrm{cvg}})})} \leqslant \delta^{\mathrm{Sc}}$$

Numerics: NLSE imaginary time with Semi-Implicit Euler

CSWR conv. rate for NLSE eigenfunct. (theory):

$$L_{\mathrm{C}}^{\mathrm{IT}}(\tau) \approx \exp\Big(-\varepsilon\Big[\sqrt{2|\tau|} - \frac{1}{\sqrt{2|\tau|}}\big(V(0)+\kappa|\phi_\ell(0)|^2\big)\Big]\Big)$$

Ground state: $V(x) = x^2/2, \kappa = 250$ & Overlap $(-\Delta x/2, \Delta x/2)$

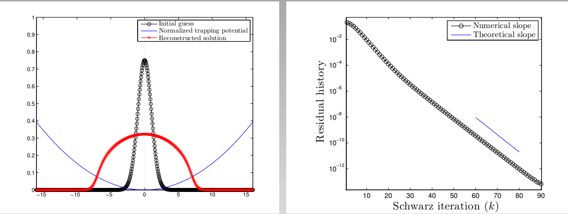
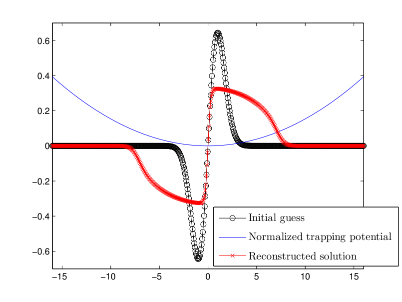


Figure : (left) Pot., Init., Recon. sol. (right) Conv. rate. Interf. at $x \approx 0$

Use: τ = time frequency - numerically $|\tau_{\mathrm{num.}}| \in [1/T^{(\mathrm{cvg})}, 1/\Delta t]$

Numerics: NLSE imaginary time

First excited state: slower convergence as $\phi_1(0) = 0$ (while $\phi_0(0) \neq 0$)



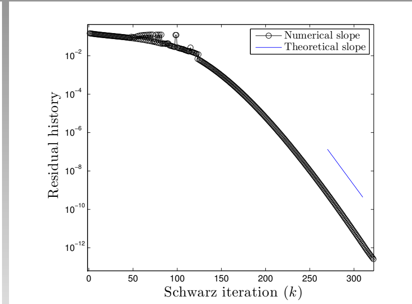
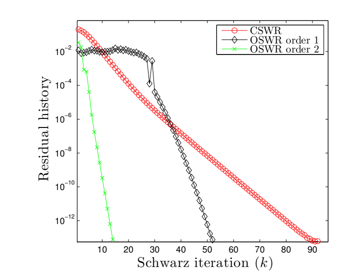


Figure : Recons. sol., trapping potential, initial guess for: (left) ground state. (right) Convergence rate. Interface at $x \approx 0$

Numerics: NLSE imaginary time

Convergence rate comparison (ground state): CSWR, M–OSWR



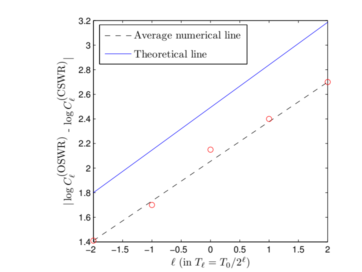


Figure : (Left) Convergence rate: CSWR vs M–OSWR (Right) $M = 1$ (DtN)

Estimate $L^{\mathrm{IT}}_{\mathrm{O;M}}(\tau) \approx c_\varepsilon^M |\tau|^{-(M+1)} L^{\mathrm{IT}}_{\mathrm{C}}(\tau)$, numer. validated [X. Antoine, E. Lorin, Numerische Math., 2017]

Numerics: LSE real time

Convergence rate in *real time* for CSWR

$$i\partial_t\psi = -\triangle\psi + V(x)\psi, \qquad \psi_0(x) = e^{-(x-a)^2+ik_0x} + e^{-(x-b)^2-ik_0x}$$

And $V(x) = -20e^{-5(x-5/2)^2}$, $T = 1$, and a, b, k_0 given.

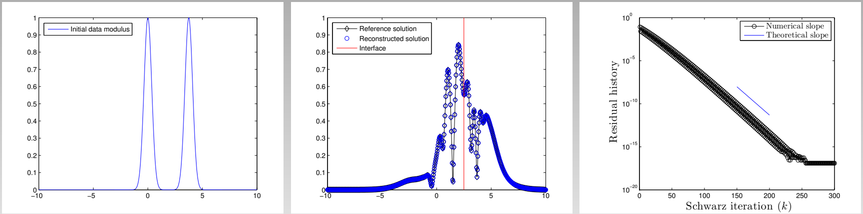


Figure : (Left) Init. data (Middle) Reconstructed sol. (Right) Conv. rate

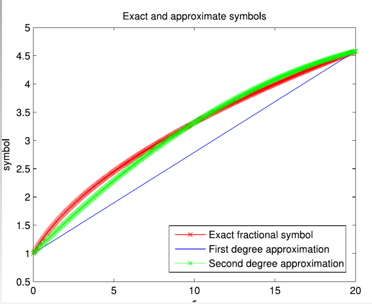
Lagrange SWR

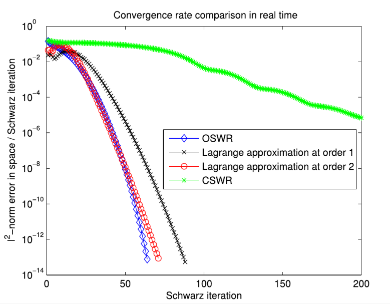
From nonlocal trans. op.... to local one...

- Approx. $\sigma(\Lambda^{\pm})$ by Lagrange poly. For instance at order 2

$$\Lambda^{\pm}(x,\partial_t) \approx L_2^{\pm}(x,\partial_t) = \pm\Big(\sqrt{V(x)} - \mathtt{i}\alpha(x)\partial_t - \beta(x)\partial_t^2\Big)$$

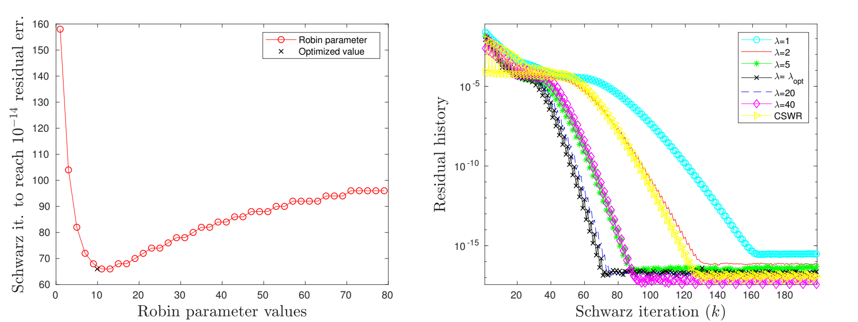
for some α, β functions. See [X. Antoine, E. Lorin, Applied Math. Lett. '16]





Optimized SWR methods

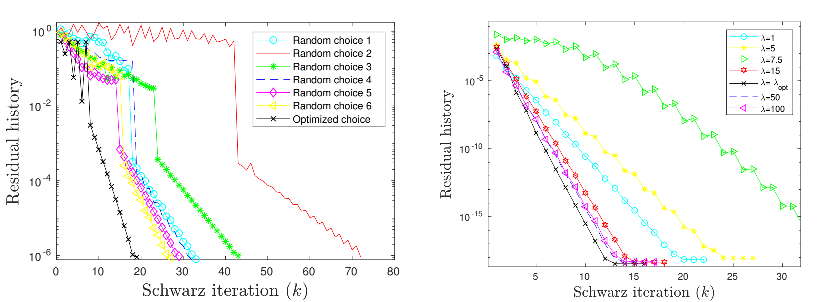
Optimized with $\Lambda^{\pm} \approx \lambda^{\pm}_{\mathrm{Opt.}}$ in Robin T.C.



Imaginary time for NLSE; [X. Antoine, E. Lorin, CiCP '19]

Optimized SWR methods

Optimized Schwarz: Multi-subdomains (8) & 2d

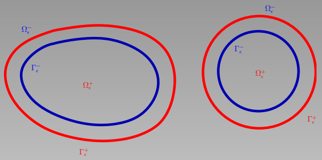


Convergence rate for NLSE in imaginary time

Two-dimensional LSE/NLSE

Extension to domain with *smooth bound.* and *non-symm.* potential

$$\mathrm{i}\partial_t\phi = -\triangle\phi + V(\mathbf{x})\phi \qquad (+\nu|\phi|^2\phi), \qquad \mathbf{x}\in\mathbb{R}^2,\ t>0$$



Convergence for CSWR

Theorem

Assuming that $\phi_0\in H^1(\Omega)$, V *is smooth,* $\Gamma_\varepsilon^\pm$ *are smooth curves then, the CSWR iterates* $(\phi^{-,(k)},\phi^{+,(k)})$ *with* $B^\pm = Id$, *exist in* $\left(H^{2,1}(\Omega_\varepsilon^\pm\times(0,T))\right)^2$.

Two-dimensional LSE/NLSE

Convergence rate estimate for CSWR - same strategy as in 1d.

Theorem (Antoine, Lorin '18)

Assume i) V smooth & bounded radial dependent, ii) sequence $\{T^{(k)}\}_k$ **decreasing** *&* **convergent** *to $0 < T^{(cvg)} < +\infty$. Then:*

$$\|((e^{C,+})^{2k+1},(e^{C,-})^{2k+1})\|_{H^{2,1}(\Omega_\varepsilon^{+}\times(0,T^{(k_0)}))\times H^{2,1}(\Omega_\varepsilon^{-}\times(0,T^{(k_0)}))} \leqslant D\big(C_\varepsilon^{C}\big)^{k}\|(h_\varepsilon^{+,0},h_\varepsilon^{-,0})\|_{\left(H^{3/4}(0,T^{(k_0)})\right)^2}$$

where D constant, and from null initial guess in $\Omega_\varepsilon^{\pm}$.

Two-dimensional LSE/NLSE

Contraction factor for CSWR

$$C_\varepsilon^C \approx \sup_{s,\tau}\Big\{|\tau|^{1/4}\frac{1}{\sqrt{2\varepsilon}}\exp\Big(-\frac{s^2}{8\varepsilon}\sqrt{2|\tau|}\Big)+\varepsilon\frac{\kappa^2(s)}{2}\frac{1}{\sqrt{2|\tau|}}\Big)$$
$$\times\exp\Big(-\frac{1}{\sqrt{2|\tau|}}\int_{-\varepsilon/2}^{\varepsilon/2}V_r(r',s)dr'\Big)\Big\}$$

with

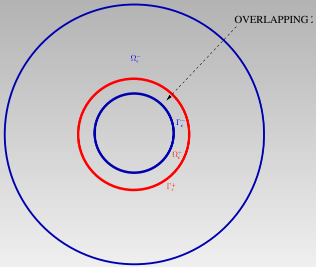
- s curvilinear abscissa
- κ local curvature

Details: X. Antoine, E. Lorin, ESAIM M2AN. '18

Two-dimensional LSE/NLSE

Example:

- $V(x,y) = \frac{1}{2}(x^2+y^2) + 4e^{-((x-1)^2+y^2)}$ and $\kappa = 200$
- 2 circular subdomains (internal: red, external: blue)
- Imaginary time method with Semi-Implicit Euler



Two-dimensional LSE/NLSE

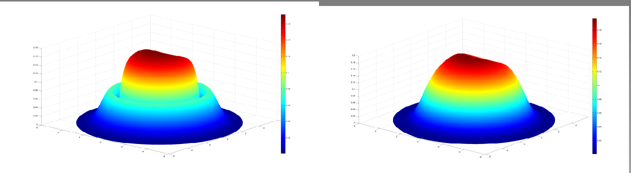


Figure : 2-d non-symmetric pot.: first Schwarz iter. and conv. sol.

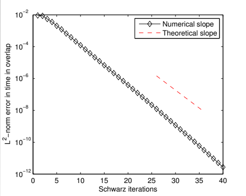


Figure : Convergence rate comparison theo. VS num.

N-body Schrödinger equation

Exact Schrödinger (not approximate models... N small)

- *Stationary* N-body problem ($3N$-dimensions)

$$H_0\psi(\mathbf{x}_1,\cdots,\mathbf{x}_N) = \lambda\psi(\mathbf{x}_1,\cdots,\mathbf{x}_N)$$

With Schrödinger Hamiltonian

$$H_0 = -\frac{1}{2}\sum_{i=1}^{N}\triangle_i - \sum_{i=1}^{N}\sum_{A=1}^{P}\frac{Z_A}{|\mathbf{x}_i - \mathbf{X}_A|} + \sum_{i=1}^{N}\sum_{j>i}^{N}\frac{1}{|\mathbf{x}_i - \mathbf{x}_j|}$$

- DD of $3N$-dim. domain in "small" $3N$-dim.subdom.
- *Time dependent* with external field $\mathbf{A}$.

$$\mathrm{i}\partial_t\psi = \Big[H_0 + \mathrm{i}\mathbf{A}(t)\sum_{i=1}^{N}\nabla_i\Big]\psi$$

Use Galerkin + Gaussian (or local Slater's deter.) basis funct..

N-body Schrödinger equation

SWR-DDM of dN−dim. space. Ex: $N = 2$ and $d = 1$

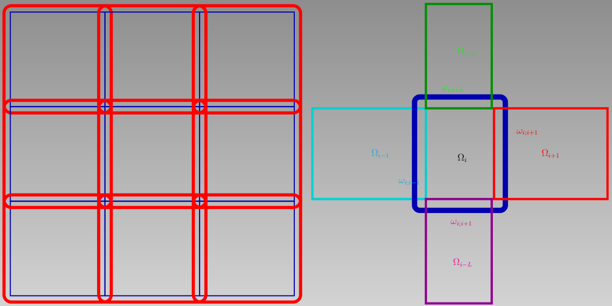


Figure : (Left) Overlapping subdomains in red. Blue subdomains do not overlap. (Right) Domain decomposition with overlapping regions

N-body Schrödinger equation: imaginary time

Define for $K_i \in \mathbb{N}^*$ local basis functions in subdomain Ω_i

$$\phi_i^{(k)}(\cdot,t) = \sum_{j=1}^{K_i} c_j^{i,(k)}(t) v_j^i$$

with $\{v_j^i\}_{1\leqslant j\leqslant K_i}$ local basis functions. In each Ω_i solve:

$$\left\{\begin{array}{ccl}
\partial_t \phi_i^{(k)} & = & -H_0\phi_i^{(k)}, \qquad (\mathbf{x},t) \in \Omega_i \times (t_n, t_{n+1}),\\
\mathcal{B}_{i;j}\phi_i^{(k)} & = & \mathcal{B}_{i;j}\phi_j^{(k-1)}, \qquad (\mathbf{x},t) \in \Gamma_{i;j} \times (t_n, t_{n+1}),\\
\phi_i^{(k)}(\cdot,0) & = & \phi_0, \qquad \mathbf{x} \in \Omega_i,\\
\phi_i^{(k)}(\cdot,t_{n+1}) & = & \phi_i^{(k)}(\cdot,t_{n+1}^+) = \dfrac{\phi_i^{(k)}(\cdot,t_{n+1}^-)}{\|\sum_{j=1}^{LdN}\tilde{\phi}_j^{(k)}(\cdot,t_{n+1}^-)\|_2}, \qquad \mathbf{x} \in \Omega_i
\end{array}\right.$$

N-body Schrödinger equation

In practice

- Use Robin Transmission Conditions $\mathcal{B}_{i;j}$ with $\mu_{ij} > 0$:

$$\big(\partial_{\mathbf{n}_{ij}} + \mathrm{i}\mu_{ij}\big)\psi_i^{(k)} = \big(\partial_{\mathbf{n}_{ij}} + \mathrm{i}\mu_{ij}\big)\psi_j^{(k-1)}, \qquad (\mathbf{x}, t)\Gamma_{i;j} \times (0, T)$$

- Convergence criteria: for all $i \neq j$ in $\{1, \cdots, L^{dN}\}$ by

$$\Big\| \sum_{i=1}^{L^{dN}} \big\| \phi_{i|\Gamma_{i;j}}^{\mathrm{cvg},(k)} - \phi_{j|\Gamma_{i;j}}^{\mathrm{cvg},(k)} \big\|_{L^2(\Gamma_{i;j})} \Big\|_{L^2(0, T^{(k^{\mathrm{cvg}})})} \leqslant \delta^{\mathrm{Sc}}. \qquad (1)$$

- Scaling: solve *in parall.* *many* small lin. syst. rather than 1 big (many small discrete Hamiltonian not a huge one!)
- *Multilevel*: *coarse* → *fine* preconditioning for convergence acceleration [X. Antoine, E. Lorin, Applied Math. & Comput., '18].

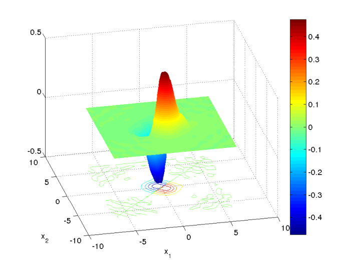
N-body Schrödinger equation

Embarrassingly parallel algo. & for $1 < \beta \leqslant 3$, L^{dN} subdom.

- **Stationary case**. *Efficient if*: $\sum_{k=1}^{k^{(\mathrm{cvg})}} N^{(k)} \ll L^{dN(\beta-1)}$, where $N^{(k)}$ NGF iterations
- **Time-dependent case**. *Efficient if*: $k^{(\mathrm{cvg})} \ll L^{dN(\beta-1)}$

N-body Schrödinger equation

So far... implemented *only* in $N = 2, d = 1$...



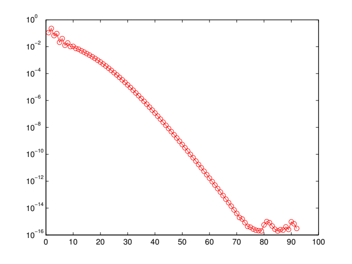


Figure : H_2-molecule ground state: 25 subdomains. (Left) Antisymmetric wavefunction. (Right) Residual error.

See also some time-dependent tests in [E. Lorin, Numer. Algo., 2019]

Conclusion

- Choice *transmission conditions* in SWR: compromise between
  1. Fast CV of SWR... and
  2. ... efficient/stable approx. of transmission operator
  3. Ex: CSWR, Robin, Lagrange-SWR, OSWR...
- Analysis strategy valid
  - Real/imaginary time: in symbols $\mathtt{i}t \mapsto t$, $\mathtt{i}\tau \mapsto \tau$
  - Other type of (wave) equations (Dirac to do !)
  - Higher dimension with smooth bound...
  - Analysis for multi-subdomain problems
- Applications in (slow) progress (N-body Schrödinger)...

Numerics: NLSE imaginary time

Semi-implicit-Euler for NGF/NLSE 1-d

$$\begin{cases} \left(\frac{I}{\Delta t} - \partial_x^2 + V(x) + \kappa|\phi^{\pm,n,(k)}|^2\right)\widetilde{\phi}^{\pm,n+1,(k)} = \frac{\phi^{\pm,n,(k)}}{\Delta t}, \text{ in } \Omega^{\pm}_{a,\varepsilon}, \\ \left(\partial_{\mathbf{n}^{\pm}} + \sqrt{\frac{2}{\Delta t}}\right)\widetilde{\phi}^{\pm,n+1,(k)}_{\pm\varepsilon/2} = g^{\mp,n+1,(k-1)}_{\pm\varepsilon/2} + \alpha^{\pm,n,(k)}_{\pm\varepsilon/2} - \alpha^{\mp,n,(k-1)}_{\pm\varepsilon/2}, \\ \widetilde{\phi}^{\pm,n+1,(k)} = 0, \text{ at } x = \mp a. \end{cases} \tag{2}$$

At each iteration $(n+1,k)$, global sol. $\widetilde{\phi}^{n+1,(k)}$ is normalized

$$\phi^{n+1,(k)} := \frac{\widetilde{\phi}^{+,n+1,(k)} + \widetilde{\phi}^{-,n+1,(k)}}{\|\widetilde{\phi}^{+,n+1,(k)} + \widetilde{\phi}^{-,n+1,(k)}\|_{L^2((-a,a))}}$$

Numerics: NLSE imaginary time

$$g^{\mp,n+1,(k-1)}_{\pm\varepsilon/2} = \partial_{\mathbf{n}^{\pm}} \widetilde{\phi}^{\mp,n+1,(k-1)}_{\pm\varepsilon/2} + \sqrt{\frac{2}{\Delta t}} \widetilde{\phi}^{\mp,n+1,(k-1)}_{\pm\varepsilon/2},$$

$$\alpha^{\mp,n,(k)}_{\pm\varepsilon/2} = -\sqrt{\frac{2}{\Delta t}} E^{\mp,n,(k)}_{\pm\varepsilon/2} \sum_{\ell=0}^{n} \beta_{n+1-\ell} \overline{E}^{\mp,\ell,(k)}_{\pm\varepsilon/2} \widetilde{\phi}^{\mp,\ell,(k)}_{\pm\varepsilon/2},$$

$$E^{\mp,n,(k)}_{\pm\varepsilon/2} = \exp\Big(-\Delta t \sum_{q=0}^{n} (V_{\pm\varepsilon/2} + \kappa|\phi^{\mp,q,(k)}_{\pm\varepsilon/2}|^2)\Big)$$

NGF at Schwarz iteration $k \to T^{(k)}$

$$\|\phi^{n+1,(k)} - \phi^{n,(k)}\|_\infty \leqslant \delta,$$

Convergence criterion for Schwarz DDM

$$\Big\| \; \|\phi^{+,\mathrm{cvg},(k)}_{|\Gamma_\varepsilon} - \phi^{-,\mathrm{cvg},(k)}_{|\Gamma_\varepsilon}\|_{\infty,\Gamma_\varepsilon} \Big\|_{L^2(0,T^{(k^{\mathrm{cvg}})})} \leqslant \delta^{\mathrm{Sc}}$$

Convergence SWR algorithm in imaginary time

Imag. time SWR for NLSE. At *each Schwarz it.* & from (t_n, t_{n+1})

$$
\left\{
\begin{array}{lll}
\big[\partial_t - \triangle + V\big]\widetilde{\phi}^{\pm,(k)} & = & 0,\ (x,t) \in \Omega_\varepsilon^{\pm} \times (t_n, t_{n+1}), \\
\widetilde{\phi}^{\pm,(k)}(\cdot, 0) & = & 0,\ x \in \Omega_\varepsilon^{\pm}, \\
B^{\pm}\widetilde{\phi}^{\pm,(k)}\big(\pm\varepsilon/2, \cdot\big) & = & B^{\pm}\widetilde{\phi}^{\mp,(k-1)}\big(\pm\varepsilon/2, \cdot\big),\ t \in (t_n, t_{n+1}) \\
\phi^{(k)}(\cdot, t_{n+1}) & = & \dfrac{\widetilde{\phi}^{+,(k)}(\cdot, t_{n+1}) + \widetilde{\phi}^{-,(k)}(\cdot, t_{n+1})}{\|\widetilde{\phi}^{+,(k)}(\cdot, t_{n+1}) + \widetilde{\phi}^{-,(k)}(\cdot, t_{n+1})\|_{L^2(\mathbb{R})}}
\end{array}
\right.
$$

- *Each* Schwarz it. k solve NGF minimization prob. in $T^{(k)}$
- $\Rightarrow$ 2 levels of convergence: Schwarz + NGF