Influence of gauges in the time dependent Ginzburg-Landau model[1]

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[1] C. Tain, J-G. Caputo and I. Danaila, *Influence of gauges in the numerical simulation of the TDGL model*. On arxiv, 2024.

Sommaire

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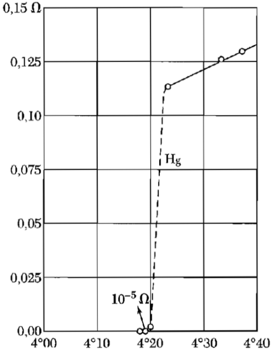

Sommaire

Non-dimensionalized Ginzburg-Landau Gibbs free energy[1]

$$\mathcal{G}(\psi, \mathbf{A}) = \int_\Omega \underbrace{\frac{1}{2}\left(|\psi|^2 - 1\right)^2}_{\text{condensation energy}} + \underbrace{\left|\left(\frac{1}{\kappa}\nabla - i\mathbf{A}\right)\psi\right|^2}_{\text{kinetic energy}} + \underbrace{|\mathbf{curl}\,\mathbf{A} - \mathbf{H}|^2}_{\text{magnetic energy}}. \qquad (1)$$

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Unknowns

- ψ is the order parameter.
  $|\psi|^2$ corresponds to the density of superconducting charges.
  We have $|\psi| \leq 1$ ($|\psi| = 0$ corresponds to the **normal** state, $|\psi| = 1$ to the pure **superconducting** state).
- $\mathbf{A}$ is the magnetic vector potential.
- ϕ is the electric potential.

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Data

- κ is the Ginzburg-Landau parameter.
- $\mathbf{H}$ is the applied magnetic field.

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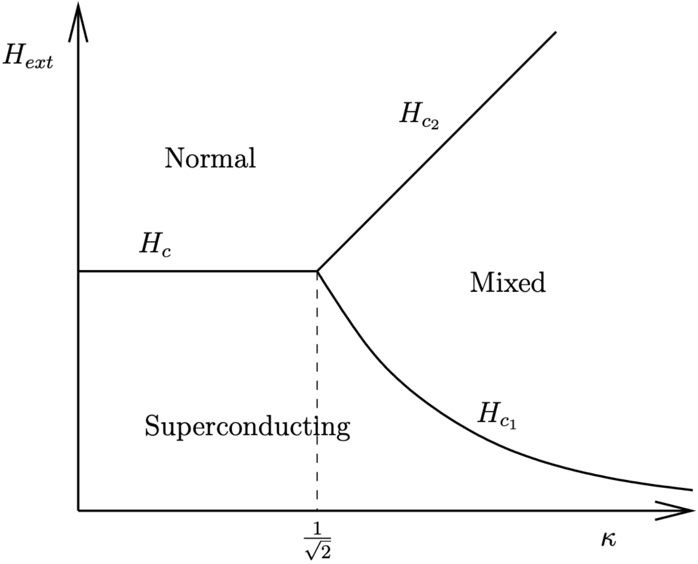
Phase diagram of a superconducting material



Non-dimensionalized TDGL system [1]

The model reads

$$\frac{\partial \psi}{\partial t} + i\kappa\phi\psi = -\frac{1}{2}\frac{\partial \mathcal{G}}{\partial \psi}(\psi, \mathbf{A}),$$
$$\frac{\partial \mathbf{A}}{\partial t} + \nabla\phi = -\frac{1}{2}\frac{\partial \mathcal{G}}{\partial \mathbf{A}}(\psi, \mathbf{A}),$$

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with boundary and initial conditions

$$\left(\frac{1}{\kappa}\nabla - i\mathbf{A}\right)\psi \cdot \mathbf{n} = 0 \text{ on } \partial\Omega,$$
$$\mathbf{curl}\,\mathbf{A} \times \mathbf{n} = \mathbf{H} \times \mathbf{n} \text{ on } \partial\Omega.$$

$$\psi(\mathbf{x}, 0) = \psi_0(\mathbf{x}) \text{ in } \Omega,$$
$$\mathbf{A}(\mathbf{x}, 0) = \mathbf{A}_0(\mathbf{x}) \text{ in } \Omega.$$

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- → In the numerics, the initial state is the pure superconducting state ($\psi_0 = 1$, $\mathbf{A}_0 = \mathbf{0}$).
- → If we take $\phi = 0$ (the temporal gauge), we see that the TDGL system corresponds to a usual descent gradient method.

[1] L.P. Gorkov and G.M. Eliashburg *Generalization of the GL equations for non-stationary problems in the case of alloys with paramagnetic impurities.* Sov. Phys. (JETP). 1968.

Computing the derivatives $\frac{\partial \mathcal{G}}{\partial \psi}$, $\frac{\partial \mathcal{G}}{\partial \mathbf{A}}$ we arrive at

$$\left(\frac{\partial}{\partial t} + i\kappa\phi\right)\psi = \left(\frac{1}{\kappa}\nabla - i\mathbf{A}\right)^2 \psi + \psi - |\psi|^2\psi \text{ in } \Omega,$$
$$\left(\frac{\partial \mathbf{A}}{\partial t} + \nabla\phi\right) = -\,\mathbf{curl}\,(\mathbf{curl}\,\mathbf{A} - \mathbf{H}) + \frac{1}{2i\kappa}(\psi^*\nabla\psi - \psi\nabla\psi^*) - |\psi|^2\mathbf{A} \text{ in } \Omega,$$

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Gauge choice

- → The solution of the TDGL is not unique.
- → A solution is defined up to a gauge transformation:

$$G_\chi(\psi, \mathbf{A}, \phi) = (\zeta, \mathbf{Q}, \Theta),$$

where $\zeta = \psi e^{i\kappa\chi}, \quad \mathbf{Q} = \mathbf{A} + \nabla\chi, \quad \Theta = \phi - \frac{\partial \chi}{\partial t},$

and χ is any function.

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→ The most common choices of gauge are

- $\phi = 0$: temporal gauge,
- $\text{div}(\mathbf{A}) = 0$: Coulomb gauge,
- $\phi = -\text{div}(\mathbf{A})$: Lorenz gauge.

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$\Longrightarrow$ Linked with the ω-gauge [1]: $\phi = -\omega \mathrm{div}(\mathbf{A})$.

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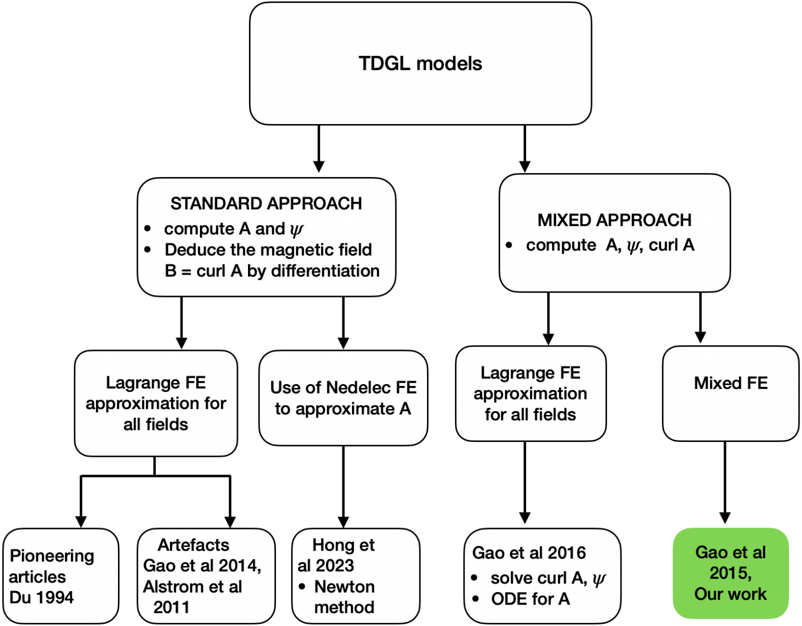
TDGL models
STANDARD APPROACH
• compute A and ψ
• Deduce the magnetic field B = curl A by differentiation
MIXED APPROACH
• compute A, ψ, curl A
Lagrange FE approximation for all fields
Use of Nedelec FE to approximate A
Lagrange FE approximation for all fields
Mixed FE
Pioneering articles Du 1994
Artefacts Gao et al 2014, Alstrom et al 2011
Hong et al 2023
• Newton method
Gao et al 2016
• solve curl A, ψ
• ODE for A
Gao et al 2015, Our work

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  - $\rightarrow$ to compute physically relevant quantities (e.g. the magnetic field $\mathbf{curl}\,\mathbf{A}$ instead of only $\mathbf{A}$),
  - $\rightarrow$ to look for a weaker formulation when standard formulations fail due to a lack of regularity of the solution.

The Poisson equation on a L-shape domain

Consider we want to solve in 2D

$$\mathbf{curl}\,\mathrm{curl}\,\mathbf{A} - \nabla\,\mathrm{div}\,\mathbf{A} = \mathbf{f}, \text{ in } \Omega, \quad \mathbf{A}\cdot\mathbf{n} = 0, \quad \mathrm{curl}\,\mathbf{A} = 0, \quad \text{on } \partial\Omega. \tag{2}$$

- $-\nabla\,\mathrm{div}\,\mathbf{A} + \mathbf{curl}\,\mathrm{curl}\,\mathbf{A} = -\Delta\mathbf{A}$ is called the Hodge Laplacian.

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- The variational formulation is

$$\int_\Omega \mathrm{curl}\,\mathbf{A}\cdot\mathrm{curl}\,\mathbf{v} + \int_\Omega \mathrm{div}\,\mathbf{A}\,\mathrm{div}\,\mathbf{v} = \int_\Omega \mathbf{f}\cdot\mathbf{v}. \tag{3}$$

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- The field $\mathbf{A}$ is necessarily approximated by Lagrange finite elements (i.e. continous).

→ *Problem:* this method will fail when the solution has a singularity (e.g. on a non-convex domain).

Instead we set $\gamma = \operatorname{curl} \mathbf{A}$ and solve

$$\mathbf{curl}\,\gamma - \nabla \operatorname{div} \mathbf{A} = \mathbf{f}, \text{ in } \Omega, \quad \mathbf{A} \cdot \mathbf{n} = 0, \quad \gamma = 0, \quad \text{on } \partial\Omega. \tag{4}$$

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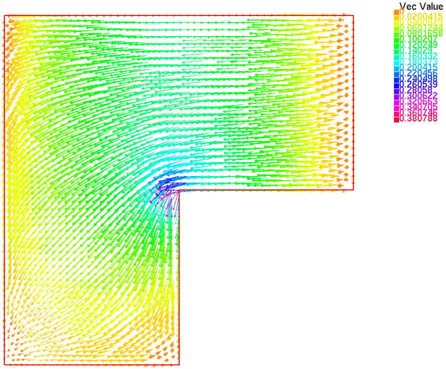
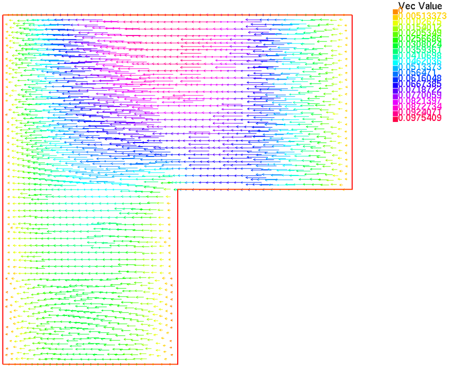
- The Sobolev space to consider is: $(\gamma, \mathbf{A}) \in \mathrm{H}_0^1 \times \mathrm{H}_0(\operatorname{div})$
- γ is approximated by **Lagrange** finite element and **A** by **Raviart-Thomas** finite elements.

→ This method will succeed and capture the singularity of the solution.

Mixed FEM (left) and Lagrange FEM (right)





Variational formulation in 2D [1]

$$\frac{\partial \psi}{\partial t} - i\kappa\omega \mathrm{div}(\mathbf{A}) = -\left(\frac{i}{\kappa}\nabla + \mathbf{A}\right)^2 \psi + \psi - |\psi|^2\psi, \tag{7}$$

$$\gamma = \mathrm{curl}\,\mathbf{A}, \tag{8}$$

$$\frac{\partial \mathbf{A}}{\partial t} - \omega\nabla \mathrm{div}(\mathbf{A}) + \mathbf{curl}\,\gamma = \frac{1}{2i\kappa}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right) - |\psi|^2\mathbf{A} + \mathbf{curl}\,H. \tag{9}$$

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$$\left(\frac{\partial \psi}{\partial t}, w\right) - i\kappa\omega\left((\mathrm{div}(\mathbf{A})\psi, w\right) = -\left(\left(\frac{1}{\kappa}\nabla - i\mathbf{A}\right)\psi, \left(\frac{1}{\kappa}\nabla - i\mathbf{A}\right)w\right) \tag{10}$$
$$+ \left(\left(1 - |\psi|^2\right)\psi, w\right) \quad \forall w \in \mathcal{H}^1(\Omega),$$

$$(\gamma, \chi) - (\mathbf{curl}\,\chi, \mathbf{A}) = 0 \quad \forall \chi \in \mathrm{H}_0^1(\Omega),$$

$$\left(\frac{\partial \mathbf{A}}{\partial t}, \mathbf{v}\right) + (\mathbf{curl}\,\gamma, \mathbf{v}) + (\omega\,\mathrm{div}\,\mathbf{A}, \mathrm{div}\,\mathbf{v}) - \frac{1}{2i\kappa}\left(\psi^*\nabla\psi - \psi\nabla\psi*, \mathbf{v}\right) \tag{11}$$

$$+ (|\psi|^2\mathbf{A}, \mathbf{v}) = (\mathbf{curl}\,H, \mathbf{v}) \quad \forall \mathbf{v} \in \mathbf{H}_0(\mathrm{div}, \Omega)). \tag{12}$$

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Discretization scheme in 2D [1]

- ψ^{n+1} in V_h^r (Lagrange FE),
- γ^{n+1} in V_h^{r+1},
- $\mathbf{A}^{n+1}$ in $\overset{\circ}{RT}_{h,r}$ (Raviart-Thomas FE),

$$\frac{1}{\delta t}(\psi^{n+1}, w) + \frac{1}{\kappa^2}(\nabla\psi^{n+1}, \nabla w) = \frac{1}{\delta t}(\psi^n, w) + \left(i\left(\kappa\omega + \frac{1}{\kappa}\right)\mathrm{div}(\mathbf{A}^n)\psi^n, w\right) \tag{13}$$

$$+\left(2\frac{i}{\kappa}\psi^n\mathbf{A}^n, \nabla w\right) + 1 - \mathbf{A}_n^2 - |\psi^n|^2 \text{ for all } w \text{ in } V_h^r, \tag{14}$$

$$(\gamma^{n+1}, \chi) - (\mathbf{curl}\,\chi, \mathbf{A}^{n+1}) = 0 \text{ for all } \chi \text{ in } \overset{\circ}{V}{}_h^{r+1}, \tag{15}$$

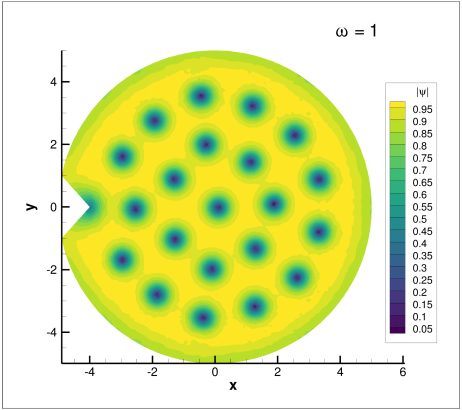
$$\frac{1}{\delta t}(\mathbf{A}^{n+1}, \mathbf{v}) + (\omega\mathrm{div}(\mathbf{A}^{n+1}), \mathrm{div}(\mathbf{v})) + (\mathbf{curl}\,\gamma^{n+1}, \mathbf{v}) = (\mathbf{curl}\,H, \mathbf{v}) \tag{16}$$

$$+\frac{1}{2i\kappa}(\psi_n^*\nabla\psi_n - \psi_n\nabla\psi_n^*, \mathbf{v}) - (|\psi^n|^2\mathbf{A}^n, \mathbf{v}) \text{ for all } \mathbf{v} \text{ in } \overset{\circ}{RT}_{h,r}. \tag{17}$$

[1] Gao, H. and Sun, W. *An efficient fully linearized semi-implicit Galerkin-mixed FEM for the dynamical Ginzburg–Landau equations of superconductivity.* JCP, 2015.

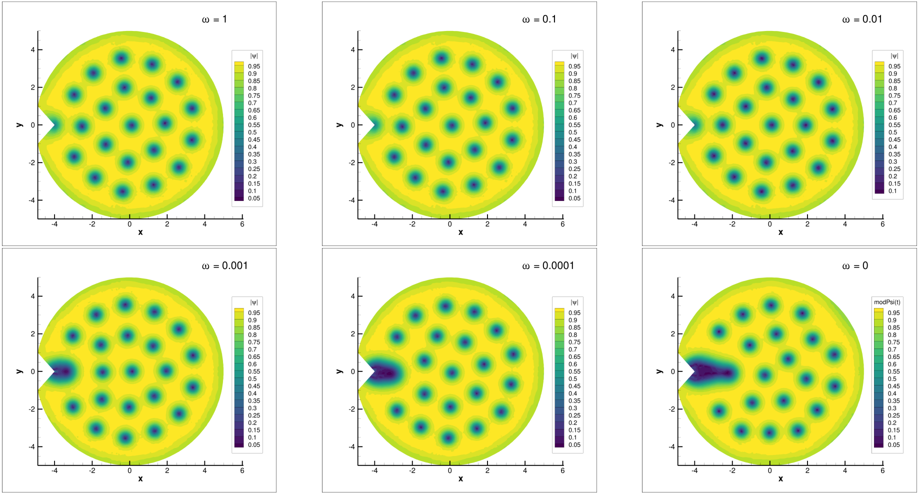
Sommaire

Finite element of order $r = 1$ under the Lorenz gauge, contours of $|\psi|$ at $t = 5000$.

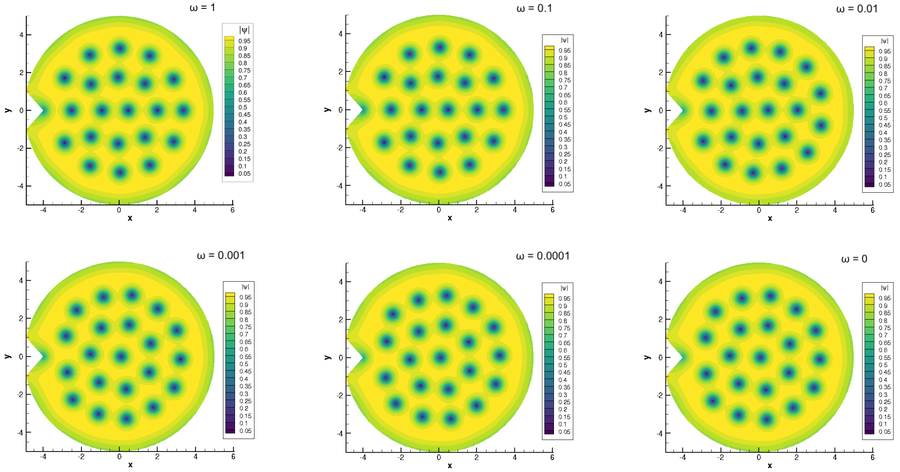


$\Rightarrow$ **Movie**

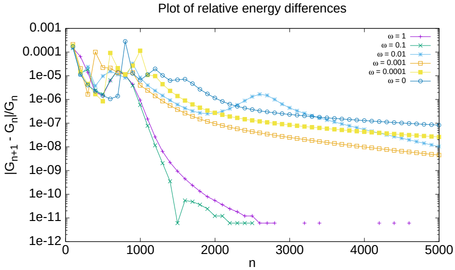
Finite element of order $r = 1$, contours of $|\psi|$ at $t = 5000$ for different values of the ω parameter



Finite element of order $r = 2$, contours of $|\psi|$ at $t = 5000$ for different values of the ω parameter

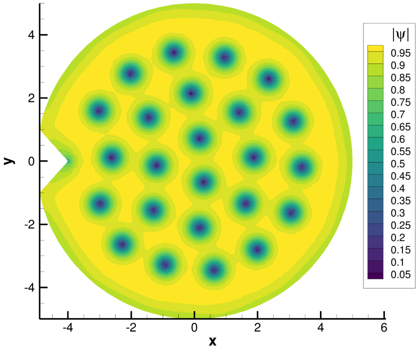


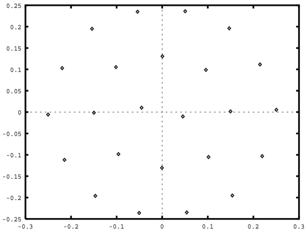
Finite element of order $r = 2$. Relative energy difference $|\mathcal{G}_{n+1} - \mathcal{G}_n|/\mathcal{G}_n$ (left) and characteristics of the vortex patten (right).



ω	Number of vortices	$\mathcal{G}_{n_{max}}$
1	21	16.4711
10^{-1}	21	16.4711
10^{-2}	22	16.0959
10^{-3}	21	16.4362
10^{-4}	21	16.4310
0	21	16.4338

Configuration of lowest energy with 24 vortices (left). Minimizer corresponding to a system of 24 point vortices [1] [2](right)





$$w_n(x_1, \ldots, x_n) = -\pi \sum_{i \neq j} \log|x_i - x_j| + C\pi n \sum_{i=1}^{n} |x_i|^2.$$

[1] Gueron, S. and Shafrir, I. *On a discrete variational problem involving interacting particles.* SIAM. 1999.

[2] Sandier, E. and Serfaty, S. *Vortices in the magnetic Ginzburg-Landau model.* Springer Science. 2008.

Manufactured system

- $\rightarrow$ Extra source term.
- $\rightarrow$ An exact solution given by an analytic expression.
- $\rightarrow$ Not physically realistic, but allows to verify the computations.

$$\frac{\partial \psi}{\partial t} - i\kappa\omega \mathrm{div}(\mathbf{A}) - \left(\frac{1}{\kappa}\nabla - i\mathbf{A}\right)^2 \psi - \psi + |\psi|^2\psi = g,$$

$$\frac{\partial \mathbf{A}}{\partial t} - \omega\nabla \mathrm{div}(\mathbf{A}) + \mathbf{curl}\,\mathrm{curl}\,\mathbf{A} - \frac{1}{2i\kappa}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right) + |\psi|^2\mathbf{A} = \mathbf{curl}\,H + \mathbf{f}.$$

$$\psi = \exp(-t)\left(\cos(\pi x) + i\cos(\pi y)\right), \tag{18}$$

$$\mathrm{A} = \begin{pmatrix} \exp(y-t)\sin(\pi x) \\ \exp(x-t)\sin(\pi y) \end{pmatrix}, \tag{19}$$

$$H = \exp(x-t)\sin(\pi y) - \exp(y-t)\sin(\pi x). \tag{20}$$

Convergence orders with a graphical method

Theoretical error estimates for the Lorenz gauge [1]

If the solution is regular enough, then

$$||\psi_h^N - \psi^N||_{L_2} = O(\Delta t + \Delta x^{r+1}),$$
$$||\mathbf{A}_h^N - \mathbf{A}^N||_{L_2} = O(\Delta t + \Delta x^{r+1}),$$
$$\Delta t \sum_{n=1}^{N} ||\gamma_h^n - \mathbf{curl}\,\mathbf{A}^n||_{L_2}^2 = O(\Delta t^2 + \Delta x^{2r+2}),$$

where r is the finite element order.

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Convergence orders with a graphical method

Theoretical error estimates for the Lorenz gauge [1]

If the solution is regular enough, then

$$||\psi_h^N - \psi^N||_{L_2} = O(\Delta t + \Delta x^{r+1}),$$
$$||\mathbf{A}_h^N - \mathbf{A}^N||_{L_2} = O(\Delta t + \Delta x^{r+1}),$$
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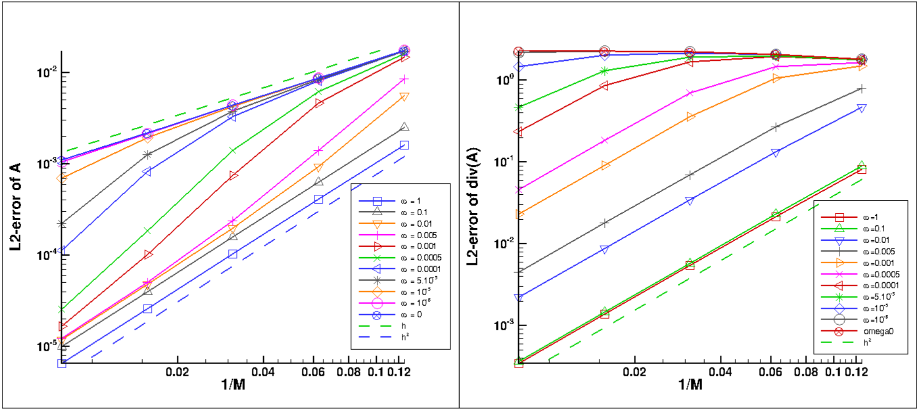
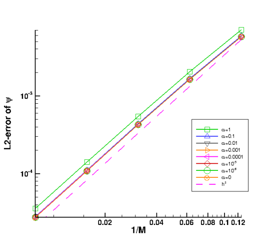
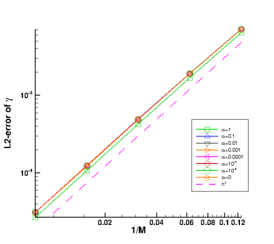
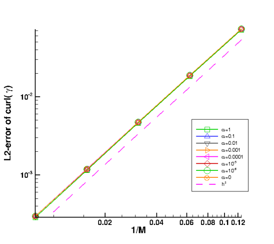
2D manufactured solutions. Finite elements of order r = 1. Orders for the vector potential **A** (left) and its divergence div **A**(right).



2D manufactured solutions. Finite elements of order r = 1. Orders for ψ, curl $\mathbf{A}$ and **curl** γ







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- Refining the mesh lead to a better convergence for each ω.
- The orders of convergence of the magnetic field and the order parameter are unaffected by the gauge.

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Strength

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Solution

- **Richardson extrapolation** method allows fast calculations and determines the order completely a priori.

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- **Principle:** for a method of order p we have

$$u_{ex} = u_h + Ch^p,$$
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We deduce

$$p = \frac{1}{\log 2}\log\left(\frac{u_{\frac{h}{2}} - u_h}{u_{\frac{h}{4}} - u_{\frac{h}{2}}}\right). \qquad (21)$$

2D manufactured solutions. Finite elements of order r = 1. Orders computed with the Richardson technique for a mesh size $\frac{1}{M} = 0.0625$.

	$\omega = 1$	$\omega = 10^{-1}$	$\omega = 10^{-2}$	$\omega = 10^{-3}$	$\omega = 10^{-4}$	$\omega = 0$
Err_{ψ}	1.99594	1.99294	1.99083	1.98507	1.9919	1.99307
$\mathrm{Err}_{\mathbf{A}}$	1.9982	1.999	2.07292	2.55124	1.36199	1.0111
Err_{γ}	2.00008	1.99683	1.99408	1.98795	1.99617	1.99735
$\mathrm{Err}_{\mathbf{curl}\,\gamma}$	2.00681	2.00412	2.00279	2.00014	2.00375	2.00425
$\mathrm{Err}_{\mathrm{div}(\mathbf{A})}$	1.99169	2.00495	2.00072	1.67622	0.941629	-0.0230222

Comparison between the Richardson method and the graphical method for the estimation of convergence orders for the vector potential **A**.

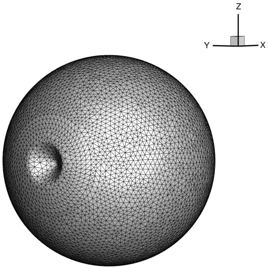
	$\omega = 1$	$\omega = 10^{-1}$	$\omega = 10^{-2}$	$\omega = 10^{-3}$	$\omega = 10^{-4}$	$\omega = 0$
Richardson	1.9982	1.999	2.0729	2.5512	1.3619	1.0111
Graphic	1.9893	1.9897	2.1514	2.7523	1.6501	0.9982

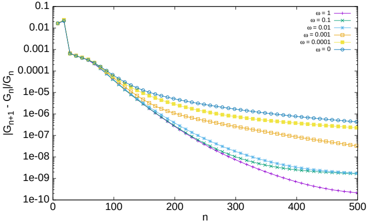
Sommaire

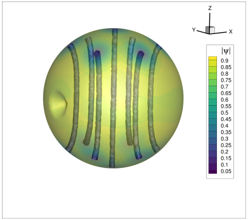
A sphere with a geometrical defect

Parameters

- $\mathbf{H} = (0, 0, 5)$,
- $\kappa = 10$,
- Number of nodes per unit ξ : 3,
- $\Delta t = 0.1$,
- Final time : $T = 500$.







Movie

Sommaire

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- We analysed the link between the choice of a gauge and the behaviour of a mixed scheme for the TDGL model.
- We demonstrated the existence of a tipping-point value for the gauge parameter.
- We presented the Richardson method, a fast and reliable alternative to the graphical method.

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