# Structure preserving discretization of Maxwell's equations with a staggered-grid mimetic spectral element method

William Barham[1,2], Philip J. Morrison[2]
Oden Institute for Computational Engineering and Sciences[1],
Department of Physics and Institute for Fusion Studies[2],
The University of Texas at Austin

Yaman Güçlü[3], Eric Sonnendrücker[3,4]
Max-Plank-Institut für Plasmaphysik[3]
& Technische Universität München, Zentrum Mathematik[4]

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# Macroscopic Maxwell: vector calculus formulation

Let $K$ be a functional of $(\boldsymbol{E}, \boldsymbol{B})$. It was shown in Morrison 2013 that the Hamiltonian

$$H[\boldsymbol{E}, \boldsymbol{B}] = K - \int_\Omega \boldsymbol{E} \cdot \frac{\delta K}{\delta \boldsymbol{E}} \, \mathrm{d}\boldsymbol{x} + \frac{1}{8\pi} \int_\Omega (\boldsymbol{E} \cdot \boldsymbol{E} + \boldsymbol{B} \cdot \boldsymbol{B}) \, \mathrm{d}\boldsymbol{x}$$

along with Poisson bracket

$$\{F, G\} = 4\pi c \int_\Omega \left[ \frac{\delta F}{\delta \boldsymbol{D}} \cdot \nabla \times \frac{\delta G}{\delta \boldsymbol{B}} - \frac{\delta G}{\delta \boldsymbol{D}} \cdot \nabla \times \frac{\delta F}{\delta \boldsymbol{B}} \right] \, \mathrm{d}\boldsymbol{x}$$

gives rise to the macroscopic Maxwell equations where the polarization and magnetization are $\boldsymbol{P} = -\delta K / \delta \boldsymbol{E}$ and $\boldsymbol{M} = -\delta K / \delta \boldsymbol{B}$ respectively.

# Equations of motion and constitutive relations

The first step is to rewrite the equations in terms of differential forms:

$$\begin{aligned} \partial_t \boldsymbol{B} &= -c\nabla \times \boldsymbol{E}, \\ \partial_t \boldsymbol{D} &= c\nabla \times \boldsymbol{H}, \\ \nabla \cdot \boldsymbol{B} =&0, \ \nabla \cdot \boldsymbol{D} = 0 \end{aligned} \quad \Longleftrightarrow \quad \begin{aligned} \partial_t \boldsymbol{b}^2 &= -c\mathrm{d}\boldsymbol{e}^1, \\ \partial_t \tilde{\boldsymbol{d}}^2 &= c\mathrm{d}\tilde{\boldsymbol{h}}^1, \\ \mathrm{d}\boldsymbol{b}^2 =&0, \ \mathrm{d}\tilde{\boldsymbol{d}}^2 = 0. \end{aligned}$$

where

$$\begin{aligned} \boldsymbol{D} &= \boldsymbol{E} - 4\pi\frac{\delta K}{\delta \boldsymbol{E}} \\ \boldsymbol{H} &= \boldsymbol{B} + 4\pi\frac{\delta K}{\delta \boldsymbol{B}} \end{aligned} \quad \Longleftrightarrow \quad \begin{aligned} \tilde{\boldsymbol{d}}^2 &= \star\boldsymbol{e}^1 - 4\pi\frac{\tilde{\delta} K}{\delta \boldsymbol{e}^1} \\ \tilde{\boldsymbol{h}}^1 &= \star\boldsymbol{b}^2 + 4\pi\frac{\tilde{\delta} K}{\delta \boldsymbol{b}^2}. \end{aligned}$$

# Hamiltonian formulation using differential forms

In terms of differential forms, the Hamiltonian may be written

$$H[\boldsymbol{e}^1, \boldsymbol{b}^2] = K - \int_\Omega \boldsymbol{e}^1 \wedge \star \frac{\delta K}{\delta \boldsymbol{e}^1} + \frac{1}{8\pi} \int_\Omega \left( \boldsymbol{e}^1 \wedge \star \boldsymbol{e}^1 + \boldsymbol{b}^2 \wedge \star \boldsymbol{b}^2 \right),$$

and the Poisson bracket may be written

$$\{F, G\} = 4\pi c \left[ \int_\Omega \frac{\tilde{\delta} F}{\delta \tilde{\boldsymbol{d}}^2} \wedge \mathrm{d} \frac{\tilde{\delta} G}{\delta \boldsymbol{b}^2} - \int_\Omega \frac{\tilde{\delta} G}{\delta \tilde{\boldsymbol{d}}^2} \wedge \mathrm{d} \frac{\tilde{\delta} F}{\delta \boldsymbol{b}^2} \right].$$

These give rise to the previously stated macroscopic Maxwell equations: $\dot{F} = \{F, H\}$.

# Finite element de Rham complex

The continuous and discrete levels of the de Rham complex may be represented by the following commuting diagram:

$$
\begin{tikzcd}
\cdots \arrow[r] & V^k \arrow[r, "\mathrm{d}_k"] \arrow[d, "\boldsymbol{\sigma}_k"] \arrow[dd, bend right, "\Pi_k"'] & V^{k+1} \arrow[r] \arrow[d, "\boldsymbol{\sigma}_{k+1}"'] \arrow[dd, bend left, "\Pi_{k+1}"] & \cdots \\
& \mathcal{C}^k \arrow[r, "\mathbb{d}_k"] \arrow[d, "\mathcal{I}_k"] & \mathcal{C}^{k+1} \arrow[d, "\mathcal{I}_{k+1}"'] & \\
\cdots \arrow[r] & V_h^k \arrow[r, "\mathrm{d}_k"] & V_h^{k+1} \arrow[r] & \cdots
\end{tikzcd}
$$

A similarly defined dual de Rham complex of twisted differential forms is defined. The two are related by the Hodge star operator.

# Two notions of duality

We may define two duality pairings on the double de Rham complex:

$$\left(\omega^k, \eta^k\right) = \int_M \omega^k \wedge \star\eta^k \quad \left\langle \tilde{\omega}^{n-k}, \eta^k \right\rangle = \int_M \tilde{\omega}^{n-k} \wedge \eta^k.$$

We may define functional derivatives with respect to each duality pairing:

$$DK[\omega^k]\delta\omega^k = \left(\frac{\delta K}{\delta\omega^k}, \delta\omega^k\right) = \left\langle \frac{\tilde{\delta} K}{\delta\omega^k}, \delta\omega^k \right\rangle.$$

Hence, if $\omega^k \in V^k$, then $\tilde{\delta}K/\delta\omega^k \in \tilde{V}^{n-k}$.

# Discrete Hodge star operator

By restricting to finite element subspaces, we can define a Hodge star operator which acts as a projection between the straight and twisted complexes:

$$\boldsymbol{u}_h^k = \star_{k,n-k}\tilde{\boldsymbol{u}}_h^{n-k} \iff \left\langle \eta^k, \tilde{\boldsymbol{u}}_h^{n-k} \right\rangle = \left(\eta^k, \boldsymbol{u}_h^k\right) \quad \forall \eta^k \in V_h^k$$
$$\tilde{\boldsymbol{v}}_h^k = \tilde{\star}_{k,n-k}\boldsymbol{v}_h^{n-k} \iff \left\langle \tilde{\chi}^k, \boldsymbol{v}_h^{n-k} \right\rangle = \left(\tilde{\chi}^k, \tilde{\boldsymbol{v}}_h^k\right) \quad \forall \tilde{\chi}^k \in \tilde{V}_h^k.$$

At the coefficient level this may be expressed as:

$$\mathbf{u}^k = \star_{k,n-k}\tilde{\mathbf{u}}^{n-k} = \mathbb{M}_k^{-1}\mathbb{M}_{k,n-k}\tilde{\mathbf{u}}^{n-k}$$
$$\tilde{\mathbf{v}}^k = \tilde{\star}_{k,n-k}\mathbf{v}^{n-k} = \tilde{\mathbb{M}}_k^{-1}\tilde{\mathbb{M}}_{k,n-k}\mathbf{v}^{n-k}.$$

# Discrete duality

Duality between the two complexes at the coefficient level may be summarized in the following diagram:

$$
\begin{tikzcd}
\mathcal{C}_k \arrow[r, shift left, "\mathbb{M}_k"] \arrow[d, "\mathbb{d}_k"] & \tilde{\mathcal{C}}^*_k \arrow[l, shift left, "\mathbb{M}_k^{-1}"] & \tilde{\mathcal{C}}_{n-k} \arrow[l, "\mathbb{M}_{k,n-k}"'] \\
\mathcal{C}_{k+1} \arrow[r, shift left, "\mathbb{M}_{k+1}"] & \tilde{\mathcal{C}}^*_{k+1} \arrow[l, shift left, "\tilde{\mathbb{M}}_{k+1}^{-1}"] \arrow[u, "\mathbb{d}_k^T"'] & \tilde{\mathcal{C}}_{n-(k+1)} \arrow[l, "\mathbb{M}_{k+1,n-(k+1)}"'] \arrow[u, "\tilde{\mathbb{d}}_{n-(k+1)}"']
\end{tikzcd}
$$

A similar diagram describes projection from the straight complex onto the twisted complex.

# Discrete functional derivatives

The above mathematical framework allows us to discretize functional derivatives in a structure preserving manner.

For $K : \Lambda^k \to \mathbb{R}$, and $\mathsf{K} = K \circ \mathcal{I}_k$,

$$\frac{\tilde{\delta} K \circ \Pi_k}{\delta u^k} = \tilde{\mathcal{I}}_{n-k} \frac{\partial \mathsf{K}}{\partial \mathbf{u}_*^k} + O(\|I - \Pi_k\|)$$

where $\mathbf{u}_*^k := \tilde{\mathbb{M}}_{n-k,k} \boldsymbol{\sigma}_k(u^k) = \tilde{\mathbb{M}}_{n-k,k} \mathbf{u}^k$.

These discrete variational derivatives can be used to directly discretize the Hamiltonian structure of the macroscopic Maxwell equations.

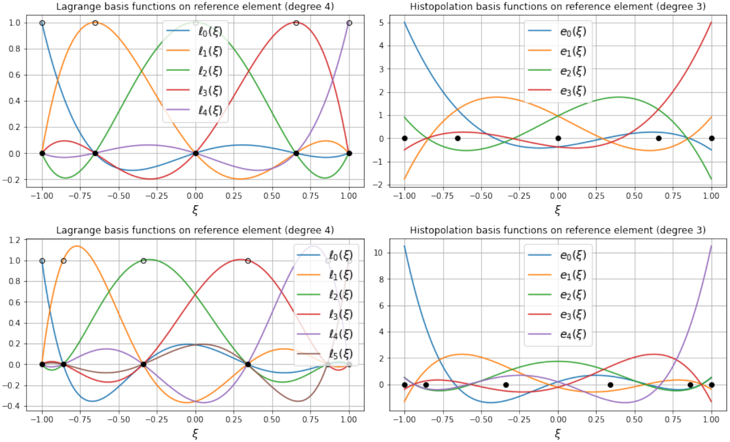
# Double de Rham complex in 1D

In 1D, the double de Rham complex may be visualized with the following diagram:

$$
\begin{tikzcd}
V^0 = H^1 \arrow[r, "\boldsymbol{\sigma}_0"] \arrow[d, "\mathsf{d}_0 = \partial_x"] & \mathcal{C}^0 \arrow[r, shift left, "\tilde{\star}_{10}"] \arrow[d, "\mathbb{d}_0"] & \tilde{\mathcal{C}}_1^* \arrow[l, shift left, "\star_{01}"] & \tilde{V}^1 = H^1 \arrow[l, "\tilde{\boldsymbol{\sigma}}_1"'] \\
V^1 = L^2 \arrow[r, "\boldsymbol{\sigma}^1"] & \mathcal{C}^1 \arrow[r, shift left, "\tilde{\star}_{10}"] & \tilde{\mathcal{C}}^0 \arrow[l, shift left, "\star_{10}"] \arrow[u, "\tilde{\mathbb{d}}_0"'] & \tilde{V}^0 = L^2 \arrow[l, "\tilde{\boldsymbol{\sigma}}_0"'] \arrow[u, "\tilde{\mathsf{d}}_0 = -\partial_x"']
\end{tikzcd}
$$

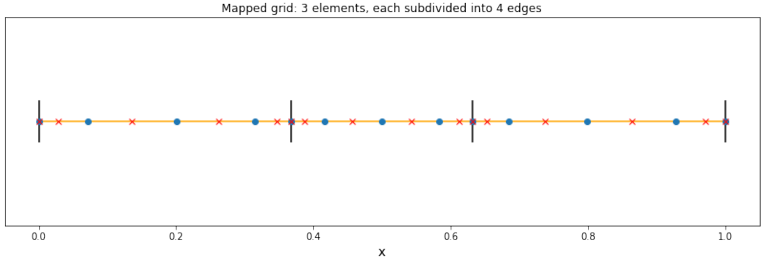
The discrete Hodge star operators are in general rectangular and hence non-invertible.

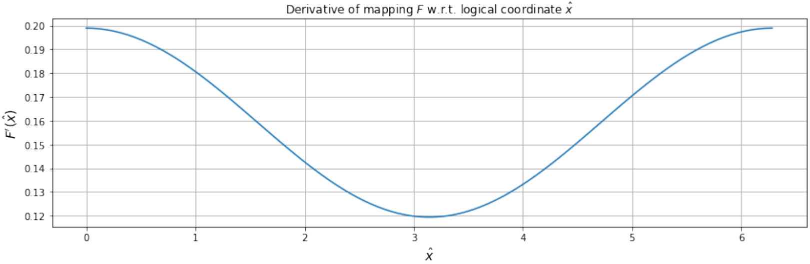
# Shape functions in 1D




The shape functions $\ell_i(\xi)$ are used to interpolate 0-forms, and $e_i(\xi)$ are used to interpolate 1-forms. Twisted forms are interpolated over a grid which is staggered with respect to that which interpolates straight forms.

# Mapped grids in 1D



# Discrete equations of motion

We discretize the equations by applying the degrees of freedom operator:

$$\begin{aligned}\tilde{\boldsymbol{\sigma}}^2\left(\partial_t \tilde{\boldsymbol{d}}^2\right) &= \tilde{\boldsymbol{\sigma}}^2\left(\mathrm{d}\tilde{\boldsymbol{h}}^1\right) \\ \boldsymbol{\sigma}^2\left(\partial_t \boldsymbol{b}^2\right) &= \boldsymbol{\sigma}^2\left(-\mathrm{d}\boldsymbol{e}^1\right)\end{aligned} \quad \Longleftrightarrow \quad \begin{aligned}\partial_t \tilde{\mathbf{d}}^2 &= \tilde{\mathbb{d}}_1 \tilde{\mathbf{h}}^1 \\ \partial_t \mathbf{b}^2 &= -\mathbb{d}_1 \mathbf{e}^1\end{aligned}$$

where $\tilde{\mathbf{d}}^2 = \tilde{\boldsymbol{\sigma}}^2\left(\tilde{\boldsymbol{d}}^2\right)$, $\tilde{\mathbf{h}}^1 = \tilde{\boldsymbol{\sigma}}^1\left(\tilde{\boldsymbol{h}}^1\right)$, $\mathbf{b}^2 = \boldsymbol{\sigma}^2\left(\boldsymbol{b}^2\right)$, and $\mathbf{e}^1 = \boldsymbol{\sigma}^1\left(\boldsymbol{e}^1\right)$. The discretized constitutive relations become

$$\begin{aligned}\mathbb{M}_1 \mathbf{e}^1 - 4\pi \frac{\partial \mathsf{K}}{\partial \mathbf{e}^1} &= \mathbb{M}_{12} \tilde{\mathbf{d}}^2 \\ \tilde{\mathbb{M}}_1 \tilde{\mathbf{h}}^1 &= \tilde{\mathbb{M}}_{12} \mathbf{b}^2 + 4\pi \frac{\partial \mathsf{K}}{\partial (\tilde{\mathbb{M}}_{12} \mathbf{b}^2)}.\end{aligned}$$

# Discrete Hamiltonian structure

The discrete Hamiltonian is written

$$\mathsf{H} = \mathsf{K} - (\mathbf{e}^1)^T \frac{\partial \mathsf{K}}{\partial \mathbf{e}^1} + \frac{1}{8\pi}\left[(\mathbf{e}^1)^T \mathbb{M}_1 \mathbf{e}^1 + (\mathbf{b}^2)^T \mathbb{M}_{21} \tilde{\mathbb{M}}_1^{-1} \tilde{\mathbb{M}}_{12} \mathbf{b}^2\right]$$

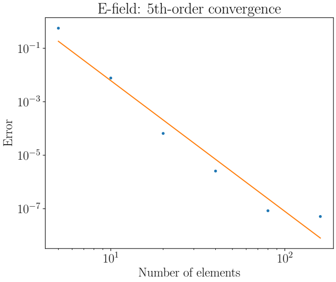
The discrete Poisson bracket is given by

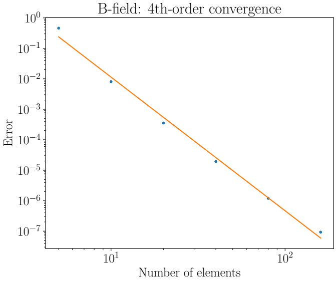
$$\{\mathsf{F}, \mathsf{G}\} = 4\pi c \left(\frac{\partial \mathsf{F}}{\partial \mathbf{d}^1_*}, \frac{\partial \mathsf{F}}{\partial \tilde{\mathbf{b}}^1_*}\right)^T \begin{pmatrix} 0 & \mathbb{M}_{12}\tilde{\mathbb{d}}_1 \\ -\tilde{\mathbb{M}}_{12}\mathbb{d}_1 & 0 \end{pmatrix} \begin{pmatrix} \partial \mathsf{G}/\partial \mathbf{d}^1_* \\ \partial \mathsf{G}/\partial \tilde{\mathbf{b}}^1_* \end{pmatrix}.$$

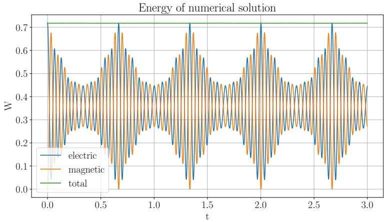
The resulting Hamiltonian system has Casimirs $\mathsf{F}[\mathbb{d}_1 \mathbb{M}_{12} \tilde{\mathbf{d}}^2]$ and $\mathsf{G}[\tilde{\mathbb{d}}_1 \tilde{\mathbb{M}}_{12} \mathbf{b}^2]$. The resulting equations of motion are

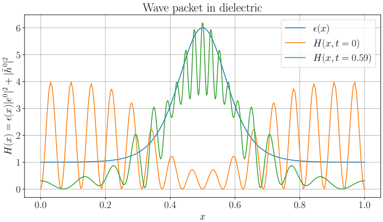
$$\mathbb{M}_{12}\left(\partial_t \tilde{\mathbf{d}}^2 - \tilde{\mathbb{d}}^1 \tilde{\mathbf{h}}^1\right) = 0, \quad \tilde{\mathbb{M}}_{12}\left(\partial_t \mathbf{b}^2 - \mathbb{d}_1 \mathbf{e}^1\right) = 0.$$

# 1D simulation results



# Acknowledgements and References

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