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MATHEMATIK

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NATURWISSENSCHAFTLICHE
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Master Thesis Introduction:

Quadrature-Free Implementation of the Local Discontinuous Garlerkin Method

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Applied Mathematics I and Computer Science 10
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Outline

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1 Problem Description and (L)DG Formulation

The Advection Problem

Model problem

Let $J := (0, t_{\text{end}})$ be a finite time interval, $\Omega \subset \mathbb{R}^2$ a polygonally bounded domain with boundary $\partial\Omega$ and outward unit normal $\boldsymbol{\nu}$.

$$
\begin{aligned}
\partial_t c(t,\boldsymbol{x}) + \boldsymbol{\nabla} \cdot (\boldsymbol{u}(t,\boldsymbol{x}) c(t,\boldsymbol{x})) &= f(t,\boldsymbol{x}) && \text{in } J \times \Omega\,,\\
c &= c_{\mathrm{D}} && \text{on } J \times \partial\Omega_{\text{in}}(t)\,,\\
c &= c^0 && \text{on } \{0\} \times \Omega\,,
\end{aligned}
$$

where $\boldsymbol{u} : J \times \Omega \to \mathbb{R}^2$, $f : J \times \Omega \to \mathbb{R}$, $c^0 : \Omega \to \mathbb{R}_0^+$, $c_{\mathrm{D}} : J \times \partial\Omega_{\text{in}}(t) \to \mathbb{R}_0^+$, $\partial\Omega_{\text{in}}(t) := \{\boldsymbol{x} \in \partial\Omega | \boldsymbol{u}(t,\boldsymbol{x}) \cdot \boldsymbol{\nu} < 0\}$.

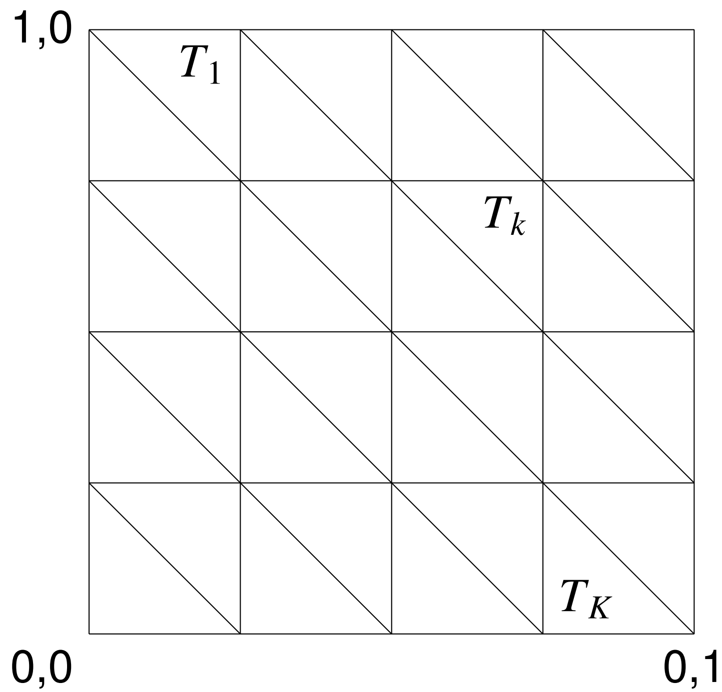
Domain decomposition

Triangulation and notation

$\mathcal{T}_h = \{T\}$ regular family of non-overlapping partitions of Ω into K closed triangles T of characteristic size h, $\overline{\Omega} = \bigcup T$. $\boldsymbol{\nu}_T$ is the exterior unit normal on ∂T.

$\mathcal{E} = \mathcal{E}_\Omega \cup \mathcal{E}_{\partial\Omega} = \{E\}$ are the sets of all edges, interior edges, and boundary edges, respectively.

One-sided values on interior edge $E \in \mathcal{E}_\Omega$ shared by triangles T^-, T^+: $w^\pm(\boldsymbol{x}) := \lim_{\varepsilon\to 0^+} w(\boldsymbol{x} - \varepsilon\boldsymbol{\nu}_{T^\pm})$



Friedrichs-Keller-Triangulation of the unit square.

LDG Discretisation

Model problem
$$\partial_t c + \boldsymbol{\nabla} \cdot (\boldsymbol{u} c) = f$$

$\longrightarrow \oplus \longleftarrow$

Triangulation
$$\mathcal{T}_h = \{T\}, \mathcal{E} = \{E\}$$

LDG Discretisation

Model problem
$\partial_t c + \boldsymbol{\nabla} \cdot (\boldsymbol{u} c) = f$

$\longrightarrow \oplus \longleftarrow$

Triangulation
$\mathcal{T}_h = \{T\}, \mathcal{E} = \{E\}$

$\downarrow$

Variational formulation

Smooth test functions $w : T \to \mathbb{R}$, integration by parts over $T \in \mathcal{T}_h$:

$$\int_T w \partial_t c(t) \mathrm{d}\boldsymbol{x} - \int_T \boldsymbol{\nabla} w \cdot \boldsymbol{u}(t) c(t) \mathrm{d}\boldsymbol{x} + \int_{\partial T} w \boldsymbol{u}(t) c(t) \cdot \boldsymbol{\nu}_T \mathrm{d}s = \int_T w f(t) \mathrm{d}\boldsymbol{x}$$

LDG Discretisation

Model problem
$\partial_t c + \boldsymbol{\nabla} \cdot (\boldsymbol{u} c) = f$

Triangulation
$\mathcal{T}_h = \{T\},\ \mathcal{E} = \{E\}$

Variational formulation

Semi-discrete formulation

With broken polynomial space $\mathbb{P}_p(\mathcal{T}_h) \ := \ \left\{ w_h : \overline{\Omega} \to \mathbb{R}\,;\ \forall T \in \mathcal{T}_h,\ w_h|_T \in \mathbb{P}_p \right\}$ and $\boldsymbol{u}_h \in [\mathbb{P}_p(\mathcal{T}_h)]^2$, $f_h(t), c_h^0 \in \mathbb{P}_p(\mathcal{T}_h)$, seek $c_h(t) \in \mathbb{P}_p(\mathcal{T}_h)$ s. t. for $t \in J$ and $\forall T^- \in \mathcal{T}_h, \forall w_h \in \mathbb{P}_p(\mathcal{T}_h)$:

$$\int_{T^-} w_h \partial_t c_h(t) \mathrm{d}\boldsymbol{x} - \int_{T^-} \boldsymbol{\nabla} w_h \cdot \boldsymbol{u}_h(t) c_h(t) \mathrm{d}\boldsymbol{x} + \int_{\partial T^-} w_h^- \boldsymbol{u}(t) \cdot \boldsymbol{\nu}_{T^-} \hat{c}_h(t) \mathrm{d}s = \int_{T^-} w_h f_h(t) \mathrm{d}\boldsymbol{x}\,,$$

where
$$\hat{c}_h(t,\boldsymbol{x})\Big|_{\partial T^-} = \left\{ \begin{array}{lll} c_h^-(t,\boldsymbol{x}) & \text{if} \quad \boldsymbol{u}(t,\boldsymbol{x}) \cdot \boldsymbol{\nu}_{T^-} \geq 0 & \text{(outflow from } T^-\text{)} \\ c_h^+(t,\boldsymbol{x}) & \text{if} \quad \boldsymbol{u}(t,\boldsymbol{x}) \cdot \boldsymbol{\nu}_{T^-} < 0 \ \wedge \ \boldsymbol{x} \notin \partial\Omega_{\text{in}} & \text{(inflow into } T^- \text{ from } T^+\text{)} \\ c_{\mathrm{D}}(t,\boldsymbol{x}) & \text{if} \quad \boldsymbol{x} \in \partial\Omega_{\text{in}} & \text{(inflow into } T^- \text{ over } \partial\Omega_{\text{in}}\text{)} \end{array} \right\}$$

LDG Discretisation

Model problem
$\partial_t c + \boldsymbol{\nabla} \cdot (\boldsymbol{u} c) = f$

$\rightarrow \oplus \leftarrow$

Triangulation
$\mathcal{T}_h = \{T\}, \mathcal{E} = \{E\}$

$\downarrow$

Variational formulation

$\downarrow$

System of equations

Modal DG basis $\forall k \in \{1, \ldots, K\}$, $\mathbb{P}_p(T_k) = \operatorname{span}\{\varphi_{ki}\}_{i \in \{1,\ldots,N_p\}}$, where $N := N_p = (p+1)(p+2)/2$.

Local basis representation: $c_h(t, \boldsymbol{x})\big|_{T_k} =: \sum_{j=1}^N C_{kj}(t)\, \varphi_{kj}(\boldsymbol{x}),\ \ \boldsymbol{u}_h(t, \boldsymbol{x})\big|_{T_k} =: \sum_{j=1}^N \sum_{m=1}^2 U_{kj}^m(t)\, \boldsymbol{e}_m \varphi_{kj}(\boldsymbol{x})$,

$$\sum_{j=1}^N \partial_t C_{kj}(t) \int_{T_k} \varphi_{ki}\, \varphi_{kj}\, \mathrm{d}\boldsymbol{x} - \sum_{j=1}^N C_{kj}(t) \sum_{l=1}^N \sum_{m=1}^2 U_{kl}^m(t) \int_{T_k} \partial_{x^m} \varphi_{ki}\, \varphi_{kl}\, \varphi_{kj}\, \mathrm{d}\boldsymbol{x}$$
$$+ \int_{\partial T_{k^-}} \varphi_{k^- i} \big(\boldsymbol{u}(t) \cdot \boldsymbol{\nu}_{k^-}\big) \left\{ \begin{array}{rl} \sum_{j=1}^N C_{k^- j}(t)\, \varphi_{k^- j} & \text{if } \ \boldsymbol{u}(t) \cdot \boldsymbol{\nu}_{k^-} \geq 0 \\ \sum_{j=1}^N C_{k^+ j}(t)\, \varphi_{k^+ j} & \text{if } \ \boldsymbol{u}(t) \cdot \boldsymbol{\nu}_{k^-} < 0 \ \wedge \ \boldsymbol{x} \notin \partial\Omega_{\text{in}} \\ c_{\mathrm{D}}(t) & \text{if } \ \boldsymbol{x} \in \partial\Omega_{\text{in}} \end{array} \right\} \mathrm{d}s \ = \ \sum_{l=1}^N F_{kl}(t) \int_{T_k} \varphi_{ki}\, \varphi_{kl}\, \mathrm{d}\boldsymbol{x} \ ,$$

$$\Leftrightarrow \quad \mathbf{M}\, \partial_t \boldsymbol{C} + \big(-\mathbf{G}^1 - \mathbf{G}^2 + \mathbf{R}\big) \boldsymbol{C} = \boldsymbol{L} - \boldsymbol{K}_D \qquad \Leftrightarrow \quad \mathbf{M}\, \partial_t \boldsymbol{C}(t) + \mathbf{A}(t) \boldsymbol{C}(t) = \boldsymbol{V}(t)$$

Classical evaluation of the integrals

Assemble mass Matrix $\mathbf{M} \in \mathbb{R}^{KN \times KN}$:

$$[\mathbf{M}]_{(k-1)N+i,(k-1)N+j} := \int_{T_k} \varphi_{ki}\, \varphi_{kj}\, \mathrm{d}\boldsymbol{x}.$$

Since φ_{ki}, $i \in \{1, \ldots, N\}$ have a support only on T_k, $\mathbf{M}$ has a block diagonal structure

$$\mathbf{M} = \begin{bmatrix} \mathbf{M}_{T_1} & & \\ & \ddots & \\ & & \mathbf{M}_{T_K} \end{bmatrix} \quad \text{with} \quad \mathbf{M}_{T_k} := \int_{T_k} \begin{bmatrix} \varphi_{k1}\varphi_{k1} & \cdots & \varphi_{k1}\varphi_{kN} \\ \vdots & \ddots & \vdots \\ \varphi_{kN}\varphi_{k1} & \cdots & \varphi_{kN}\varphi_{kN} \end{bmatrix} \mathrm{d}\boldsymbol{x}\;.$$

Using (Gaussian) quadrature for the local mass matrix $\mathbf{M}_{T_k}$ the following holds:

$$\begin{aligned} [\mathbf{M}_{T_k}]_{i,j} = [\mathbf{M}]_{(k-1)N+i,(k-1)N+j} &:= \sum_{q=1}^{N_q} \omega'_q\, g_{kij}(x'_{kq}) \\ &= \sum_{q=1}^{N_q} \omega'_q \sum_{r=1}^{N} \phi_{krij}\, \varphi_{kr}(x'_{kq}) \end{aligned}$$

with $N_q > N$ the required quadrature points on T_k, weights ω'_q, the polynomial function $g_{kij}(x)$ and its local basis expansion $\sum_{r=1}^{N} \phi_{krij}\, \varphi_{kr}(x)$

Quadrature free approach

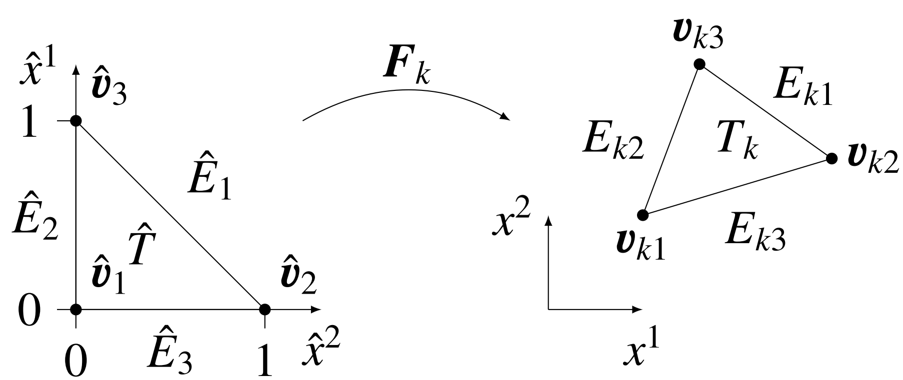
Backtransformation to the reference triangle

Transform reference triangle $\hat{T}$ to physical triangle T_k using an affine mapping

$$\boldsymbol{F}_k : \hat{T} \ni \hat{\boldsymbol{x}} \mapsto \mathbf{B}_k \hat{\boldsymbol{x}} + \boldsymbol{v}_{k1} \in T_k \quad \text{with} \quad \mathbb{R}^{2\times 2} \ni \mathbf{B}_k := \left[\boldsymbol{v}_{k2} - \boldsymbol{v}_{k1} \middle| \boldsymbol{v}_{k3} - \boldsymbol{v}_{k1} \right] .$$

For $w : \Omega \to \mathbb{R}$ we obtain **transformation formulas**

$$\int_{T_k} w(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = 2\,|T_k| \int_{\hat{T}} w \circ \boldsymbol{F}_k(\hat{\boldsymbol{x}}) \, \mathrm{d}\hat{\boldsymbol{x}} , \qquad \int_{E_{kn}} w(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = \frac{|E_{kn}|}{|\hat{E}_n|} \int_{\hat{E}_n} w \circ \boldsymbol{F}_k(\hat{\boldsymbol{x}}) \, \mathrm{d}\hat{\boldsymbol{x}} .$$



Quadrature free approach

Introducing monomial basis for polynomial expansion in the integrals

Use simple monomial basis $B_T \equiv \{\phi_{Tr}\}_{r\in 1,\dots,N_p} = \{1,\ x,\ y,\ x^2,\ xy,\ y^2,\ \dots\}$ to expand polynomials in integrals:

$$\int_T P \,\mathrm{d}\boldsymbol{x} = \int_T \sum_{r=1}^{M} p_r \phi_{Tr} \,\mathrm{d}\boldsymbol{x} = \sum_{r=1}^{M} p_r \int_T \phi_{Tr} \,\mathrm{d}\boldsymbol{x}$$

where $P \in \mathbb{P}_p(T)$, $M \geq N_p$.

Quadrature free approach

Transformation

$$\int_{T_k} w(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = 2\,|T_k| \int_{\hat{T}} w \circ \boldsymbol{F}_k(\hat{\boldsymbol{x}})\,\mathrm{d}\hat{\boldsymbol{x}}$$

$\longrightarrow \oplus \longleftarrow$

Monomial basis

$$\int_T P\,\mathrm{d}\boldsymbol{x} = \sum_{r=1}^{M} p_r \int_T \phi_{Tr}\,\mathrm{d}\boldsymbol{x}$$

Quadrature free approach

Transformation

$$\int_{T_k} w(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = 2\,|T_k| \int_{\hat{T}} w \circ \boldsymbol{F}_k(\hat{\boldsymbol{x}})\,\mathrm{d}\hat{\boldsymbol{x}}$$

$\longrightarrow \oplus \longleftarrow$

Monomial basis

$$\int_T P\,\mathrm{d}\boldsymbol{x} = \sum_{r=1}^M p_r \int_T \phi_{Tr}\,\mathrm{d}\boldsymbol{x}$$

$\downarrow$

Assembly mass matrix $\mathbf{M} \in \mathbb{R}^{KN\times KN}$

$$\begin{aligned}[\mathbf{M}]_{(k-1)N+i,(k-1)N+j} &:= \int_{T_k} \varphi_{ki}\,\varphi_{kj}\,\mathrm{d}\boldsymbol{x} \\ &= 2|T_k| \int_{\hat{T}} \hat{\varphi}_i\,\hat{\varphi}_j\,\mathrm{d}\hat{\boldsymbol{x}} \\ &= 2|T_k| \sum_{r=1}^{M} p_{ijr} b_r\end{aligned}$$

where $b_r := \int_{\hat{T}} \phi_{\hat{T}r}\,\mathrm{d}\hat{\boldsymbol{x}}$ are the analytically precomputed and stored integrals.
$M \geq N$ depends on the order of the polynomial $\varphi_{ki}\,\varphi_{kj}$.

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2 Goals of the master thesis

Goals of the master thesis

from the mathematical viewpoint

- make use of precomputed integrals of monomials
- which combinations of monomials occur?
- how to store the pre computed values efficiently?
- is it reasonable to neglect higher order monomials?
- start with linear advection problem; later non linear problems (shallow water eq.)
- use FESTUNG to test implementation

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from the computer science viewpoint

- simple C/C++ code (as baseline for code generation)
- 2D triangles on the uniformly refined unit square
- assembling the matrix **A** for the linear advection problem
- later assembling of the vector $\boldsymbol{F} - \boldsymbol{AC}$ for explicit time-stepping
- layout of the data structure for precomputed parameters p^m_{ijlr} and integrals b_r
- single core performance

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3 Appendix

Quadrature free assembly of G^{m}

Use simple monomial basis $B_T \equiv \{\phi_{Tr}\}_{r\in 1,\dots,N_p} = \{1,\ x,\ y,\ x^2,\ xy,\ y^2,\ \dots\}$ to expand polynomials in integrals:

$$\int_T P \,\mathrm{d}\boldsymbol{x} = \int_T \sum_{r=1}^{M} p_r \phi_{Tr} \,\mathrm{d}\boldsymbol{x} = \sum_{r=1}^{M} p_r \int_T \phi_{Tr} \,\mathrm{d}\boldsymbol{x}$$

where $P \in \mathbb{P}_p(T)$, $M \geq N_p$.

Quadrature free assembly of $\mathbf{G}^m$

Use simple monomial basis $B_T \equiv \{\phi_{Tr}\}_{r\in 1,\dots,N_p} = \{1,\ x,\ y,\ x^2,\ xy,\ y^2,\ \dots\}$ to expand polynomials in integrals:

$$\int_T P\,\mathrm{d}\boldsymbol{x} = \int_T \sum_{r=1}^{M} p_r \phi_{Tr}\,\mathrm{d}\boldsymbol{x} = \sum_{r=1}^{M} p_r \int_T \phi_{Tr}\,\mathrm{d}\boldsymbol{x}$$

where $P \in \mathbb{P}_p(T)$, $M \geq N_p$.

Applied in the block matrix $\mathbf{G}^m \in \mathbb{R}^{KN\times KN}, m \in \{1,2\}$ from the volume integral part:

$$\begin{aligned}
[\mathbf{G}^1]_{(k-1)N+i,(k-1)N+j} &:= \sum_{l=1}^{N} U_{kl}^1(t) \int_{T_k} \partial_{x^1}\varphi_{ki}\,\varphi_{kl}\,\varphi_{kj}\,\mathrm{d}\boldsymbol{x} \\
&= \sum_{l=1}^{N} U_{kl}^1(t) \left(\mathbf{B}_k^{2,2} \int_{\hat{T}} \partial_{\hat{x}^1}\hat{\varphi}_i\,\hat{\varphi}_l\,\hat{\varphi}_j\,\mathrm{d}\hat{\boldsymbol{x}} - \mathbf{B}_k^{2,1} \int_{\hat{T}} \partial_{\hat{x}^2}\hat{\varphi}_i\,\hat{\varphi}_l\,\hat{\varphi}_j\,\mathrm{d}\hat{\boldsymbol{x}} \right) \\
&= \sum_{l=1}^{N} U_{kl}^1(t) \sum_{r=1}^{M} \beta_{kijlr}^1 b_r
\end{aligned}$$

with $\beta_{kijlr}^1 := \mathbf{B}_k^{2,2} p_{ijlr}^1 - \mathbf{B}_k^{2,1} p_{ijlr}^1$ and analytically precomputed integrals $b_r := \int_{\hat{T}} \phi_{\hat{T}r}\,\mathrm{d}\hat{\boldsymbol{x}}$.
Analogously for for $\mathbf{G}^2$.

Assembly of mass matrix M in FESTUNG

Mass matrix $\mathbf{M} \in \mathbb{R}^{KN\times KN}$:

$$[\mathbf{M}]_{(k-1)N+i,(k-1)N+j} := \int_{T_k} \varphi_{ki}\,\varphi_{kj}\,\mathrm{d}\boldsymbol{x}.$$

Since φ_{ki}, $i \in \{1,\dots,N\}$ have a support only on T_k, $\mathbf{M}$ has a block diagonal structure

$$\mathbf{M} = \begin{bmatrix} \mathbf{M}_{T_1} & & \\ & \ddots & \\ & & \mathbf{M}_{T_K} \end{bmatrix} \quad \text{with} \quad \mathbf{M}_{T_k} := \int_{T_k} \begin{bmatrix} \varphi_{k1}\varphi_{k1} & \cdots & \varphi_{k1}\varphi_{kN} \\ \vdots & \ddots & \vdots \\ \varphi_{kN}\varphi_{k1} & \cdots & \varphi_{kN}\varphi_{kN} \end{bmatrix} \mathrm{d}\boldsymbol{x}\ .$$

For the local mass matrix holds

$$\mathbf{M}_{T_k} = 2\,|T_k|\,\hat{\mathbf{M}} \quad \text{with} \quad \hat{\mathbf{M}} := \int_{\hat{T}} \begin{bmatrix} \hat{\varphi}_1\hat{\varphi}_1 & \cdots & \hat{\varphi}_1\hat{\varphi}_N \\ \vdots & \ddots & \vdots \\ \hat{\varphi}_N\hat{\varphi}_1 & \cdots & \hat{\varphi}_N\hat{\varphi}_N \end{bmatrix} \mathrm{d}\boldsymbol{x}$$

and $\hat{\varphi}_i(\hat{\boldsymbol{x}}) = \varphi_{ki} \circ \boldsymbol{F}_k(\hat{\boldsymbol{x}})$. Hence, the global mass matrix $\mathbf{M}$ can be expressed as

$$\mathbf{M} = \begin{bmatrix} \mathbf{M}_{T_1} & & \\ & \ddots & \\ & & \mathbf{M}_{T_K} \end{bmatrix} = 2 \begin{bmatrix} |T_1| & & \\ & \ddots & \\ & & |T_K| \end{bmatrix} \otimes \hat{\mathbf{M}}\ ,$$

where $\otimes$ denotes the Kronecker product.

L2-projection of coefficient functions

We assumed $d_h(t), f_h(t), c_h^0 \in \mathbb{P}_p(\mathcal{T}_h)$.
Given an algebraic expression, e. g., for d and seek the representation matrix $\mathbf{D}(t) \in \mathbb{R}^{K \times K}$ such that

$$d_h(t, \boldsymbol{x})\Big|_{T_k} = \sum_{j=1}^{N} D_{kj}(t)\, \varphi_{kj}(\boldsymbol{x}) \ .$$

Produce d_h using the L^2 **projection** defined locally for $T_k \in \mathcal{T}_h$ by

$$\forall w_h \in \mathbb{P}_d(T)\,, \qquad \int_{T_k} w_h\, d_h(t) = \int_{T_k} w_h\, d(t) \ .$$

Time discretization

The linear system can be written as

$$\mathbf{M}\partial_t \boldsymbol{C}(t) = \boldsymbol{V}(t) - \mathbf{A}(t)\boldsymbol{C}(t) =: \boldsymbol{S}(t, \boldsymbol{C}(t))\,.$$

Discretize in time using TVD Runge–Kutta methods[1] (SSP Runge–Kutta) of orders $s \in \{1, 2, 3\}$.
Let $0 = t^1 < t^2 < \ldots t_{\mathrm{end}}$, $\Delta t^n = t^{n+1} - t^n$, $\boldsymbol{C}^n := \boldsymbol{C}(t^n)$, and $\boldsymbol{S}^{n+\delta_i} := \boldsymbol{S}(t^n + \delta_i \Delta t^n)$.

$$\begin{aligned}
\boldsymbol{C}^{(0)} &= \boldsymbol{C}^n\,, \\
\boldsymbol{C}^{(i)} &= \omega_i \boldsymbol{C}^n + (1 - \omega_i)\left(\boldsymbol{C}^{(i-1)} + \Delta t^n\,\mathbf{M}^{-1}\boldsymbol{S}^{n+\delta_i}\right)\,, \quad \text{for } i = 1, \ldots, s\,, \\
\boldsymbol{C}^{n+1} &= \boldsymbol{C}^{(s)}\,.
\end{aligned}$$

When possible, choose $s = p + 1$.

[1] S. Gottlieb, C.-W. Shu, Strong stability-preserving high-order time discretization methods, Math. Comp. 67 (221) (1998) 73–85. doi:10.1090/S0025-5718-98-00913-2