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Space-time discretisations for linear hyperbolic systems

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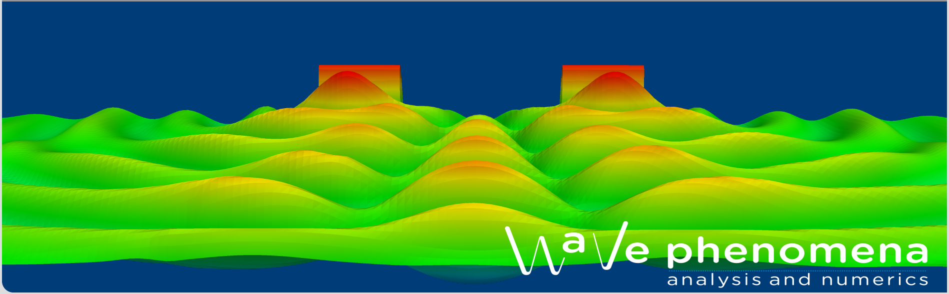

Example: The linear transport problem

The *transport equation* aims to determine a density distribution $\rho : (0, T) \times \mathbb{R}^d \to \mathbb{R}_{\geq 0}$, $d \in \{2, 3\}$, such that

$$\partial_t \rho + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{v}) = 0 \quad \text{on } \mathbb{R}^d \times (0, T)\,, \qquad \rho(\cdot, 0) = \rho_0\,,$$

for a given flow field $\boldsymbol{v} : (0, T) \times \mathbb{R}^d \to \mathbb{R}^d$ with $\boldsymbol{\nabla} \cdot \boldsymbol{v} = 0$ and initial density distribution $\rho_0 \geq 0$.

This is a conservation law with flux function

$$\boldsymbol{F} : \mathbb{R} \to \mathbb{R}^d, \quad \boldsymbol{F}(\rho) := \rho \boldsymbol{v}\,.$$

We may also read it as an abstract ODE

$$\partial_t \rho + A\rho = 0$$

with the linear operator $A\rho = \boldsymbol{\nabla} \cdot (\rho \boldsymbol{v})$.

Example: Acoustic waves

The *acoustic wave equation* describes the (small) deformation $\phi : \mathbb{R}_{\geq 0} \times \mathbb{R}^d \to \mathbb{R}$ in fluid/air by

$$\rho \partial_t^2 \phi - \kappa \Delta \phi = 0$$

in $(0, T) \times \mathbb{R}^d$ subject to initial and boundary conditions. With $p = \rho \partial_t \phi$ and $\boldsymbol{v} = \boldsymbol{\nabla} \phi$ we derive

$$\kappa^{-1} \partial_t p = \boldsymbol{\nabla} \cdot \boldsymbol{v} \quad \text{and} \quad \rho \partial_t \boldsymbol{v} = \boldsymbol{\nabla} p\,.$$

As a system in $[p, \boldsymbol{v}]$ this reads

$$\boldsymbol{0} = \begin{bmatrix} \kappa^{-1} \partial_t p \\ \rho \partial_t \boldsymbol{v} \end{bmatrix} - \begin{bmatrix} \boldsymbol{\nabla} \cdot \boldsymbol{v} \\ \boldsymbol{\nabla} p \end{bmatrix} = \begin{bmatrix} \kappa^{-1} & 0 \\ 0 & \rho \end{bmatrix} \partial_t \begin{bmatrix} p \\ \boldsymbol{v} \end{bmatrix} - \operatorname{div} \begin{bmatrix} \boldsymbol{v}^\dagger \\ p\, I_d \end{bmatrix}.$$

Thus we find the flux function

$$\boldsymbol{F} : \mathbb{R}^{d+1} \to \mathbb{R}^{d+1,d}, \quad \boldsymbol{F}\left(\begin{bmatrix} p \\ \boldsymbol{v} \end{bmatrix} \right) = - \begin{bmatrix} \boldsymbol{v}^\dagger \\ p\, I_d \end{bmatrix}.$$

As an abstract ODE it has with $\boldsymbol{u} = [p, \boldsymbol{v}]$ the form

$$M \partial_t \boldsymbol{u} + A \boldsymbol{u} = \boldsymbol{0}.$$

Example: Electromagnetic waves (1)

For a permeability μ and a permittivity ε (possibly tensor-valued) find an electric field $\boldsymbol{E}$ and a magnetic field $\boldsymbol{H}$ such that the *linear Maxwell system*

$$\mu \partial_t \boldsymbol{H} + \nabla \times \boldsymbol{E} = \boldsymbol{0}\,, \qquad \varepsilon \partial_t \boldsymbol{E} - \nabla \times \boldsymbol{H} = \boldsymbol{0}\,,$$
$$\nabla \cdot (\mu \boldsymbol{H}) = 0\,, \qquad \nabla \cdot (\varepsilon \boldsymbol{E}) = 0$$

holds for all $t \in (0, T)$ and $\boldsymbol{x} \in \mathbb{R}^3$.

This can be written as

$$L\boldsymbol{u} := M\partial_t \boldsymbol{u} + A\boldsymbol{u} = \boldsymbol{0}\,,$$

where M, A, $\boldsymbol{u}$ are given by

$$M := \begin{bmatrix} \mu & 0 \\ 0 & \varepsilon \end{bmatrix}, \quad A := \begin{bmatrix} 0 & \nabla\times \\ -\nabla\times & 0 \end{bmatrix}, \quad \boldsymbol{u} := \begin{bmatrix} \boldsymbol{H} \\ \boldsymbol{E} \end{bmatrix}.$$

Example: Electromagnetic waves (2)

There exist constant symmetric matrices $B_1, B_2, B_3 \in \mathbb{R}^{6\times 6}$ and a linear flux function $\boldsymbol{F} : \mathbb{R}^6 \to \mathbb{R}^{6,3}$ such that

$$A\boldsymbol{u} = \operatorname{div} \boldsymbol{F}(\boldsymbol{u}) = B_1\partial_{x_1}\boldsymbol{u} + B_2\partial_{x_2}\boldsymbol{u} + B_3\partial_{x_3}\boldsymbol{u}\,,$$

so we can equivalently write

$$L\boldsymbol{u} = M\partial_t\boldsymbol{u} + \operatorname{div} \boldsymbol{F}(\boldsymbol{u}) = \boldsymbol{0}\,.$$

One may simplify this problem by considering the 2D reduction

$$\boldsymbol{u} = \left[H_1, H_2, E_3\right], \quad H_3 \equiv E_1 \equiv E_2 \equiv 0\,,$$

for Maxwell's equations in $\mathbb{R}^2$ (*transverse magnetic (TM) modes*).

Second order form for $\boldsymbol{E}$ is the wave equation

$$\varepsilon\partial_t^2\boldsymbol{E} + \boldsymbol{\nabla}\times\left(\mu^{-1}\boldsymbol{\nabla}\times\boldsymbol{E}\right) = \boldsymbol{0}\,.$$

Linear hyperbolic first-order systems

For $\Omega \subset \mathbb{R}^d$ and $T > 0$ we seek $\boldsymbol{u} : (0, T) \times \Omega \subset \mathbb{R}_{\geq 0} \times \mathbb{R}^d \to \mathbb{R}^J$ such that

$$M\partial_t \boldsymbol{u}(t) + A\boldsymbol{u}(t) = \boldsymbol{f}(t) \qquad \textit{for all } t \in (0, T)\,,$$
$$\boldsymbol{u}(0) = \boldsymbol{u}_0\,,$$

with a flux function $\boldsymbol{F} : \mathbb{R}^J \to \mathbb{R}^{J,d}$ defined by

$$\boldsymbol{F}(\boldsymbol{v}) = \sum_{i=1}^{d} B_i \boldsymbol{v}\,.$$

Here $M, B_i \in \mathcal{L}^\infty(\Omega)^{J\times J}_{\text{sym}}$ and M is positive definite. Thus the operator A is given by

$$A\boldsymbol{v} = \text{div}\boldsymbol{F}(\boldsymbol{v}) = \sum_{i=1}^{d} \partial_i(B_i \boldsymbol{v}) \qquad \textit{for all } \boldsymbol{v} \in \mathcal{D}(A)\,.$$

The semigroup setting (1)

Let H be a Hilbert space with inner product $(v,w)_H$, $M : H \to H$ isomorphism, and let A be a linear operator in H with domain $\mathcal{D}(A) \subset H$.

Theorem (Existence of a semigroup)

Assume

- $\mathcal{D}(A)$ *is dense in* H,
- *there exists* $\omega \geq 0$ *with* $(Av, v)_H \geq -\omega\,(Mv, v)_H$ *for all* $v \in \mathcal{D}(A)$,
- *there exists* $\lambda_0 > \omega$ *such that* $A + \lambda_0 M$ *is onto.*

Then $-M^{-1}A$ *generates a semigroup with* $\|\exp(-tM^{-1}A)\|_H \leq \exp(\omega t)$.

If the operator $-M^{-1}A$ generates a semigroup in H, then linear evolution equation $M\partial_t u + Au = 0$ is solved by

$$u(t) = \exp(-tM^{-1}A)u(0)\,.$$

Nonhomogeneous right hand sides f can be treated with the variation of constants formula.

Evans: Partial Differential Equations

The semigroup setting (2)

Let $(\cdot,\cdot)_\Omega = \int_\Omega \ldots \,\mathrm{d}\boldsymbol{x}$.

Acoustic waves Assume $q = 0$ on $\partial\Omega$, then

$$\begin{aligned}(A[p,\mathbf{v}],[q,\mathbf{w}])_\Omega &= -(\nabla\cdot\mathbf{v},q)_\Omega - (p,\nabla\cdot\mathbf{w})_\Omega \\ &= -(\boldsymbol{\nu}\cdot\mathbf{v},q)_{\partial\Omega} - (A[q,\mathbf{w}],[p,\mathbf{v}])_\Omega \\ &= -(A[q,\mathbf{w}],[p,\mathbf{v}])_\Omega\,.\end{aligned}$$

Hence A is skew-symmetric for $q \in \mathcal{H}^1_0(\Omega)$.

Electro-magnetic waves We get that A skew-symmetric using the boundary condition $\boldsymbol{\nu}\times\boldsymbol{E} = \mathbf{0}$. Hence A is skew-symmetric for $\boldsymbol{E} \in \boldsymbol{\mathcal{H}}_0(\mathrm{curl}\Omega)$.

For the considered examples A is dissipative with $\omega = 0$.

The semigroup setting (3)

In the applications $(A+M)^{-1}$ exists and is bounded, hence $A+M$ maps onto H ($\lambda_0 = 1$).

Acoustic waves $(A+M)(p, \boldsymbol{v}) = (f, \boldsymbol{g})$ implies

$$-\Delta p + \rho\kappa^{-1} p = \rho f - \nabla\cdot\boldsymbol{g}$$

This is solvable for $p \in \mathcal{H}_0^1(\Omega)$ and $\rho\boldsymbol{v} = \boldsymbol{g} - \nabla p$.

The semigroup setting (4)

We consider a Hilbert space H with inner product $(\cdot,\cdot)_H = (M\cdot,\cdot)_\Omega$ and an operator A defined on $\mathcal{D}(A) \subset H$ to find solutions of

$$M\partial_t \boldsymbol{u} + A\boldsymbol{u} = \boldsymbol{f} \qquad \text{in } [0,T]\,.$$

Acoustic waves

$$H = \mathcal{L}^2(\Omega)\times\mathcal{L}^2(\Omega)^d, \quad M[p,\boldsymbol{v}] = [\kappa^{-1}p, \rho\boldsymbol{v}],$$
$$A[p,\boldsymbol{v}] = -[\nabla\cdot\boldsymbol{v}, \nabla p], \quad \mathcal{D}(A) = \boldsymbol{\mathcal{H}}(\mathrm{div},\Omega)\times\mathcal{H}^1_0(\Omega).$$

Electro-magnetic waves

$$H = \mathcal{L}^2(\Omega)^3\times\mathcal{L}^2(\Omega)^3, \quad M[\boldsymbol{E},\boldsymbol{H}] = [\varepsilon\boldsymbol{E}, \mu\boldsymbol{H}]\,, \quad A[\boldsymbol{E},\boldsymbol{H}] = (-\nabla\times\boldsymbol{H}, \nabla\times\boldsymbol{E})_\Omega$$
$$\mathcal{D}(A) = \big\{[\boldsymbol{E},\boldsymbol{H}] \in \boldsymbol{\mathcal{H}}_0(\mathrm{curl},\Omega)\times\boldsymbol{\mathcal{H}}(\mathrm{curl},\Omega)\colon\ \nabla\cdot(\varepsilon\boldsymbol{E}) = 0,\ \nabla\cdot(\mu\boldsymbol{H}) = 0\big\}.$$

Energy conservation

We have $(A\boldsymbol{u},\boldsymbol{w})_\Omega = -(\boldsymbol{u},A\boldsymbol{w})_\Omega$ for $\boldsymbol{u},\boldsymbol{w}\in\mathcal{D}(A)$, and this implies conservation of the energy $\mathcal{E}(\boldsymbol{u}) = \frac{1}{2}\|\boldsymbol{u}\|_V^2$, i.e., the solution satisfies

$$\partial_t\mathcal{E}(\boldsymbol{u}(t)) = 0.$$

The Babuška–Nečas setting

Theorem

Let V, W be Hilbert spaces, and let $b\colon V \times W \longrightarrow \mathbb{R}$ be a bilinear form. Assume

- *there is $C > 0$ such that for all $v \in V$, $w \in W$*

$$|b(v,w)| \le C\,\|v\|_V \|w\|_W.$$

- *there is $\beta > 0$ such that for all $v \in V$*

$$\sup_{w \in W} \frac{b(v,w)}{\|w\|_W} \ge \beta\,\|v\|_V.$$

Then, there exists for all $f \in W$ a unique solution $u \in V$ of

$$b(u,w) = (f,w)_W \qquad \text{for all } w \in W$$

that satisfies the bound $\|u\|_V \le C/\beta\,\|f\|_W$.

A space-time setting (1)

We consider now function spaces V, W, H on the space-time cylinder $Q = (0, T) \times \Omega$. Let $L = M\partial_t + A$ on Q with domain $V = \mathcal{D}(L)$, where

$$V := \overline{\{u \in \mathcal{C}^1(0, T; \mathcal{D}(A)) \,:\, u(0) = 0\}}^{\|\cdot\|_V}$$

with respect to the *weighted graph norm* ($(\cdot, \cdot)_Q = \int_Q \dots \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t$)

$$\|v\|_V^2 = (Mv, v)_Q + (M^{-1}Lv, Lv)_Q \,.$$

Then we define $W = \overline{L(V)} \subseteq H = \mathcal{L}^2(Q)^J$ with norm $\|w\|_W^2 = (Mw, w)_Q$.

Theorem

Let $(Av(\cdot), v(\cdot))_\Omega \geq 0$ a.e. for $v \in V$ (A dissipative). For given $f \in H$ there exists a unique solution $u \in V$ solving the variational problem

$$(Lu, w)_Q = (f, w)_Q \qquad \text{for all } w \in W$$

with

$$\|u\|_V \leq \sqrt{1 + 4T^2}\,\|M^{-1/2} f\|_Q \,.$$

A space-time setting (2)

Proof.
For the proof we define $b\colon V \times W \to \mathbb{R}$ with

$$b(v,w) = (Lv, w)_Q\,.$$

The continuity follows from the upper bound

$$|b(v,w)| \le \|v\|_V \|w\|_W\,.$$

We will show that for all $v \in \mathcal{C}^1(0,T;\mathcal{D}(A))$ with $v(0) = 0$

$$\|v\|_W \le 2T\,\|M^{-1}Lv\|_W\,.$$

This extends to all $v \in V$ and shows $L(V) = \overline{L(V)}$ in W. Inserting $w = M^{-1}Lv$ yields

$$\inf_{v\in V}\sup_{w\in W}\frac{b(v,w)}{\|v\|_V\|w\|_W} \ge \inf_{v\in V}\frac{b(v,M^{-1}Lv)}{\|v\|_V\|M^{-1}Lv\|_W} = \inf_{v\in V}\frac{\|M^{-1}Lv\|_W}{\sqrt{\|v\|_W^2 + \|M^{-1}Lv\|_W^2}}$$

$$\ge \frac{1}{\sqrt{1+4T^2}}\,.$$

A space-time setting (3)

To prove the stated inequality we first note that for all $\boldsymbol{v} \in \mathcal{C}^1(0,T;\mathcal{D}(A))$ with $v(0)=0$ we have

$$\begin{aligned}
\|v\|_W^2 &= \int_0^T \big(Mv(t),v(t)\big)_\Omega \,\mathrm{d}t = \int_0^T \Big(\big(Mv(t),v(t)\big)_\Omega - \big(Mv(0),v(0)\big)_\Omega\Big)\,\mathrm{d}t \\
&= \int_0^T\int_0^t \partial_t\big(Mv(s),v(s)\big)_\Omega \,\mathrm{d}s\,\mathrm{d}t = 2\int_0^T\int_0^t \big(M\partial_t v(s),v(s)\big)_\Omega \,\mathrm{d}s\,\mathrm{d}t \\
&\le 2\int_0^T\int_0^t \big(M\partial_t v(s)+Av(s),v(s)\big)_\Omega \,\mathrm{d}s\,\mathrm{d}t \\
&\le 2\int_0^T\int_0^t \big(M^{-1}Lv(s),Lv(s)\big)_\Omega^{1/2}\big(Mv(s),v(s)\big)_\Omega^{1/2} \,\mathrm{d}s\,\mathrm{d}t \\
&\le 2T\,\|M^{-1}Lv\|_W\|v\|_W\,.
\end{aligned}$$

This yields $\|v\|_W \le 2T\,\|M^{-1}Lv\|_W$ for all $v\in V$. •

Discrete space-time setting (1)

Let $V_h \subset V$ and $W_h \subset W$ be finite dimensional subspaces. Define the $\mathcal{L}^2$-projection $\Pi_h \colon W \to W_h$ by $\big(\Pi_h w, w_h\big)_Q = \big(w, w_h\big)_Q$ for $w_h \in W_h$ and $M_h = \Pi_h M$. Let $L_h \in \mathcal{L}(V_h, W_h)$ be an appropriate discrete operator with corresponding discrete bilinear form

$$b_h(v_h, w_h) = (L_h v_h, w_h)_Q .$$

We define norms

$$\|v_h\|_{V_h} = \Big(\|v_h\|_W^2 + \|M_h^{-1} L_h v_h\|_W^2\Big)^{1/2}, \quad \|w_h\|_{W_h} = \|w_h\|_W .$$

Lemma

(1) $b_h : V_h \times W_h \to \mathbb{R}$ is a continuous bilinear form.
(2) Assume that, with $d_T(t) = T - t$,

$$\big(M_h d_T \partial_t v_h, v_h\big)_Q \le \big(L_h v_h, d_T \Pi_h v_h\big)_Q \qquad \text{for all } v_h \in V_h . \tag{1}$$

Then, the bilinear form b_h is inf-sup stable on $V_h \times W_h$ with $\beta = 1/\sqrt{1 + 4T^2}$.

Discrete space-time setting (2)

Proof. (1) For all $v_h \in V_h$, $w_h \in W_h$

$$b_h(v_h, w_h) = \big(L_h v_h, w_h\big)_Q \le \|M_h^{-1} L_h v_h\|_W \|w_h\|_W \le \|v_h\|_{V_h} \|w_h\|_W \,.$$

(2) Transferring the proof of the non-discrete to the discrete setting yields

$$\begin{aligned}
\|v_h\|_W^2 &= \int_0^T \big(M_h v_h(t), v_h(t)\big)_\Omega \,\mathrm{d}t \\
&= \int_0^T \Big(\big(M_h v_h(t), v_h(t)\big)_\Omega - \big(M_h v_h(0), v_h(0)\big)_\Omega\Big) \,\mathrm{d}t \\
&= \int_0^T \int_0^t \partial_t \big(M_h v_h(s), v_h(s)\big)_\Omega \,\mathrm{d}s\,\mathrm{d}t = 2 \int_0^T \int_0^t \big(M_h \partial_t v_h(s), v_h(s)\big)_\Omega \,\mathrm{d}s\,\mathrm{d}t \\
&= 2\big(M_h \partial_t v_h, d_T v_h\big)_Q \le 2\big(L_h v_h, d_T \Pi_h v_h\big)_Q \\
&\le 2T \,\|M_h^{-1} L_h v_h\|_W \|v_h\|_W \,.
\end{aligned}$$

This yields $\|v_h\|_{V_h} \le 2T \,\|M_h^{-1} L_h v_h\|_W$. To prove the inf-sup stability we use $w_h = M_h^{-1} L_h v_h$.

Discrete space-time setting (3)

Application of the Babuška–Nečas result.

Theorem

Let b_h *be inf-sup stable on* $V_h \times W_h$ *with* $\beta = 1/\sqrt{1+4T^2}$. *Then, for given* $f \in H$ *there exists a unique solution* $u_h \in V_h$ *of*

$$(L_h u_h, w_h)_Q = (f, w_h)_Q \qquad \text{for all } w_h \in W_h\,,$$

satisfying the a priori bound $\|u_h\|_{V_h} \leq \sqrt{4T^2+1}\|M_h^{-1}\Pi_h f\|_W$.

Space–Time decomposition

Decomposition of the space-time domain $Q = (0, T) \times \Omega$:

- Decompose $(0, T)$ such that $[0, T] = \bigcup_{n=1}^{N} \overline{I_n}$, where I_n is an open interval $I_n = (t_{n-1}, t_n) \subset (0, T)$ for $n = 1, \ldots, N$.
- Decompose Ω such that $\overline{\Omega} = \bigcup_K \overline{K}$, where K is an open set (e.g. triangle).
- This defines a decomposition $\mathcal{R}$ of Q

$$\mathcal{R} = \{R = I_n \times K \,:\, n \le N,\ K \in \mathcal{K}\}.$$

- For $R = I \times K$ let $h_K = \mathrm{diam}(K)$ be the spatial mesh size and let $h_I = |I|$ be the local timestep size, and $h_R = h_I + h_K$.
- Let $\mathcal{F}_K$ be the set of faces of $K \in \mathcal{K}$.

An implicit space-time dG approximation (1)

For every $R = I \times K$ choose polynomial degrees p_R and q_R for the ansatz in space and time, and define the *local test spaces*

$$W^{h,R} = \big(\mathbb{P}_{q_R-1}(I) \times \mathbb{P}_{p_R}(K)\big)^J$$

and the *global test space*

$$W^h = \big\{\mathbf{w}^h \in \mathcal{L}^2(Q)^J \;:\; \mathbf{v}^h|_R \in W^{h,R}\big\}\,.$$

For the *ansatz space*, we choose the affine space depending on the initial condition

$$V^h = \Big\{\mathbf{v}^h \in \mathcal{H}^1(0,T;\mathcal{L}^2(\Omega)^J) \;:\; \mathbf{v}^h(0) = \mathbf{u}_0 \text{ and for all } R \in \mathcal{R} \text{ and } (t,\mathbf{x}) \in R$$

$$\mathbf{v}^h(t,\mathbf{x}) = \frac{t_n - t}{t_n - t_{n-1}}\mathbf{v}^{h,R}(t_{n-1},\mathbf{x}) + \frac{t - t_{n-1}}{t_n - t_{n-1}}\mathbf{w}^{h,R}(\mathbf{x})\,,$$

$$\text{where } \mathbf{v}^{h,R} \in V^h|_{[0,t_{n-1}]} \text{ and } \mathbf{w}^{h,R} \in W^{h,R}\Big\}\,.$$

An implicit space-time dG approximation (2)

Multiplying $A\boldsymbol{u} = \operatorname{div}\boldsymbol{F}(\boldsymbol{u})$ with a test function $\boldsymbol{w}_K$ and integrating over a spatial cell K yields

$$
\begin{aligned}
(A\boldsymbol{u}, \boldsymbol{w}_K)_{0,K} &= \int_K \operatorname{div}\boldsymbol{F}(\boldsymbol{u}) \cdot \boldsymbol{w}_K \,\mathrm{d}\boldsymbol{x} \\
&= -\int_K \boldsymbol{F}(\boldsymbol{u}) \colon \nabla \boldsymbol{w}_K \,\mathrm{d}\boldsymbol{x} + \sum_{f \in \mathcal{F}_K} \int_f \boldsymbol{F}(\boldsymbol{u}) \boldsymbol{n}_{K,f} \cdot \boldsymbol{w}_K \,\mathrm{d}\boldsymbol{x}\,.
\end{aligned}
$$

$\boldsymbol{n}_{K,f}$ denotes the outer unit normal on the face f of K with respect to K.

An implicit space-time dG approximation (3)

Given a *consistent numerical flux* $\boldsymbol{F}^{\text{num}}_{K,f}(\boldsymbol{v}^h)$ on $f \in \mathcal{F}_K$ we define $A_h\boldsymbol{v}^h \in V^h$ by

$$(A_h\boldsymbol{v}^h, \boldsymbol{w}^h_K)_{0,K} = -\int_K \boldsymbol{F}(\boldsymbol{v}^h_K) \cdot \nabla \boldsymbol{w}^h_K \,\mathrm{d}\boldsymbol{x} + \sum_{f\in\mathcal{F}_K} \int_f \boldsymbol{F}^{\text{num}}_{K,f}(\boldsymbol{v}^h)\boldsymbol{n}_{K,f} \cdot \boldsymbol{w}^h_K \,\mathrm{d}\boldsymbol{x}$$

for all $\boldsymbol{v}^h \in V^h$, $\boldsymbol{w}^h_K \in V^h_K$ and all K. This can be rewritten by partial integration as

$$(A_h\boldsymbol{v}^h, \boldsymbol{w}^h_K)_{0,K} = \int_K \operatorname{div}\boldsymbol{F}(\boldsymbol{v}^h_K) \cdot \boldsymbol{w}^h_K \,\mathrm{d}\boldsymbol{x} + \sum_{f\in\mathcal{F}_K} \int_f \big(\boldsymbol{F}^{\text{num}}_{K,f}(\boldsymbol{v}^h) - \boldsymbol{F}(\boldsymbol{v}^h_K)\big)\boldsymbol{n}_{K,f} \cdot \boldsymbol{w}^h_K \,\mathrm{d}\boldsymbol{x}\,.$$

Hesthaven and Warburton 2008

For inner faces $f \in \mathcal{F}_K$ let K_f be the neighbouring cell with $f = \partial K \cap \partial K_f$.

A numerical flux is called *consistent* if on inner faces f the difference $\big(\boldsymbol{F}^{\text{num}}_{K,f}(\boldsymbol{v}^h) - \boldsymbol{F}(\boldsymbol{v}^h_K)\big)\boldsymbol{n}_{K,f}$ only depends on $[\boldsymbol{v}_h]_{K,f} = \boldsymbol{v}_{h,K_f} - \boldsymbol{v}_{h,K}$ and that $\big(\boldsymbol{F}^{\text{num}}_{K,f}(\boldsymbol{v}) - \boldsymbol{F}(\boldsymbol{v})\big)\boldsymbol{n}_{K,f} = \boldsymbol{0}$ for $\boldsymbol{v} \in \mathcal{D}(A)$.

Upwind flux

f a planar interface with normal $\boldsymbol{n}$. Define the symmetric matrix $\boldsymbol{F_n} = \sum_i n_i B_i$. x the variable along the normal direction and define for constant vectors $\boldsymbol{u}^{\mathrm{L}}$, $\boldsymbol{u}^{\mathrm{R}}$

$$\boldsymbol{u}^0(x) = \boldsymbol{u}^{\mathrm{L}} \chi_{\{x \le 0\}} + \boldsymbol{u}^{\mathrm{R}} \chi_{\{x > 0\}} \,.$$

Solve exactly the *Riemann problem*

$$M\partial_t \overline{\boldsymbol{u}} + \partial_x \boldsymbol{F_n} \overline{\boldsymbol{u}} = \boldsymbol{0} \qquad \text{for all } t > 0,\ x \in \mathbb{R}\,,$$
$$\overline{\boldsymbol{u}}(0, \cdot) = \boldsymbol{u}^0 \,.$$

Solve the eigenvalue problem $\boldsymbol{F_n} \boldsymbol{w}^i = \lambda_i M \boldsymbol{w}^i$ and define the splitting $\boldsymbol{F_n} = \boldsymbol{F_n^+} + \boldsymbol{F_n^-}$. The numerical flux ("upwind flux") is now given by

$$\boldsymbol{F}^{\mathrm{num}}(\overline{\boldsymbol{u}}) = \boldsymbol{F_n}(\overline{\boldsymbol{u}}(t,0)) = \boldsymbol{F_n^+}(\boldsymbol{u}^{\mathrm{L}}) + \boldsymbol{F_n^-}(\boldsymbol{u}^{\mathrm{R}}) = \boldsymbol{F_n}(\boldsymbol{u}^{\mathrm{L}}) + \boldsymbol{F_n^-}(\boldsymbol{u}^{\mathrm{R}} - \boldsymbol{u}^{\mathrm{L}})$$

Thus $\boldsymbol{F}^{\mathrm{num}}(\overline{\boldsymbol{u}}) - \boldsymbol{F_n}(\boldsymbol{u}^{\mathrm{L}})$ depends on the jump $\boldsymbol{u}^{\mathrm{R}} - \boldsymbol{u}^{\mathrm{L}}$ only. This flux is consistent and non-negative

$$(A_h \boldsymbol{v}^h, \boldsymbol{v}^h)_\Omega \ge C \sum_{K \in \mathcal{K}} \sum_{f \in \mathcal{F}_K} \left\| \boldsymbol{n}_K \cdot (\boldsymbol{F}^{\mathrm{num}}(\boldsymbol{v}^h) - \boldsymbol{F}(\boldsymbol{v}_K^h)) \right\|_f^2 \,.$$

Upwind flux for linear transport

For the upwind flux we get

$$\left(A_h\rho_h\,,\,\eta_{h,K}\right)_K = \left(\boldsymbol{v}\cdot\boldsymbol{\nabla}\rho_{h,K}\,,\,\eta_{h,K}\right)_K + \sum_{f\in\mathcal{F}_K}\frac{1}{2}\left(\left(\boldsymbol{n}_K\cdot\boldsymbol{v}-|\boldsymbol{n}_K\cdot\boldsymbol{v}|\right)[\rho_h]_{K,f}\,,\,\eta_{h,K}\right)_{0,f}.$$

Upwind flux for electro-magnetic waves

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For the upwind flux we get [1]

$$
\begin{aligned}
\big(A_h(\boldsymbol{H}^h, \boldsymbol{E}^h), (\phi_K^h, \psi_K^h)\big)_{0,K} = {} & (\nabla \times \boldsymbol{E}_K^h, \phi_K^h)_{0,K} - \big(\nabla \times \boldsymbol{H}_K^h, \psi_K^h\big)_{0,K} \\
& + \sum_{f \in \mathcal{F}_K} \Big\{ \quad \frac{Z_{K_f}}{Z_K + Z_{K_f}} \big(\boldsymbol{n}_{K,f} \times [\boldsymbol{E}^h]_{K,f}, \phi_K^h\big)_{0,f} \\
& \qquad - \frac{Y_{K_f}}{Y_K + Y_{K_f}} \big(\boldsymbol{n}_{K,f} \times [\boldsymbol{H}^h]_{K,f}, \psi_K^h\big)_{0,f} \\
& \qquad + \frac{1}{Z_K + Z_{K_f}} \big(\boldsymbol{n}_{K,f} \times (\boldsymbol{n}_{K,f} \times [\boldsymbol{H}^h]_{K,f}), \phi_K^h\big)_{0,f} \\
& \qquad + \frac{1}{Y_K + Y_{K_f}} \big(\boldsymbol{n}_{K,f} \times (\boldsymbol{n}_{K,f} \times [\boldsymbol{E}^h]_{K,f}), \psi_K^h\big)_{0,f} \Big\}
\end{aligned}
$$

for $(\boldsymbol{E}^h, \boldsymbol{H}^h) \in V^h$ and $(\psi_K^h, \phi_K^h) \in V_K^h$, $Z_K := \sqrt{\mu_K/\varepsilon_K} = 1/Y_K$.

[1] E.g. Hesthaven and Warburton 2008.

Discrete space-time setting (3)

We use a tensor-product discretisation in space-time. The ansatz space consists of local polynomials of degree p, q, while the test space of those of degree $p, q-1$.

We defined a spatial operator $A_h : V_h \to W_h$ with a consistent numerical flux and with the property $(A_h v_h, v_h) \geq 0$ for all $v_h \in V_h$.

We defined the discrete space-time operator $L_h \in \mathcal{L}(V_h, W_h)$ by

$$L_h = M_h \partial_t v_h + A_h v_h$$

and the corresponding discrete bilinear form by $b_h(\cdot,\cdot) = (L_h \cdot, \cdot)_Q$.

Lemma

If the discretization has tensor product structure, the inf-sup condition for b_h holds if we have for all $v_h \in V_h$

$$\Pi_h \partial_t v_h = \partial_t v_h \,, \quad \big(M_h d_T \partial_t v_h, v_h\big)_Q \leq \big(M_h \partial_t v_h, d_T \Pi_h v_h\big)_Q \,, \quad 0 \leq \big(A_h v_h, d_T \Pi_h v_h\big)_Q \,.$$

This is fulfilled by the above construction.

Discrete space-time setting (4)

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Theorem

With the inf-sup constant β (as before) we arrive at the error estimate

$$\|u - u^h\|_{V^h} \leq \left(1 + \sqrt{1 + 4T^2}\right) \inf_{v_h \in V^h} \|u - v^h\|_{V^h} .$$

If in addition the solution is sufficiently smooth and the space-time discretisation has tensor product structure with polynomial degrees p, q (both ≥ 1), we obtain the a priori error estimate

$$\|u - u_h\|_{V_h} \leq C\left(\triangle t^q + \triangle x^p\right)\left(\|\partial_t^{q+1} u\|_Q + \|\mathrm{D}^{p+1} u\|_Q\right) .$$

Proof

Strang lemma and interpolation.

The implicit Space-Time dG Approximation

Summary

- *Ansatz space V^h: Discontinuous in space and continuous in time*
- *Test space W^h: Discontinuous in space and time*
- *Approximate continuity across faces by the upwind flux*

Advantage

- *No CFL (Courant–Friedrichs–Lewy) condition $\Rightarrow$ allows larger time intervals*
- *Parallel computation in* **space and time** *using a parallel GMRES solver with multigrid preconditioner*

Disadvantage

- *Large linear system with many unknowns $\Rightarrow$ adaptive strategy is needed*

Dual Error Estimator

- Goal: Minimise the error $e := u - u^h$ w.r.t. to a given output $\mathcal{J}(u)$.
- Use the *dual problem*

$$\left(w, L^* u_*\right)_Q = \mathcal{J}'[u](w) \qquad \textit{for all } w \in W$$

  with dual solution $u_* \in V^*$ to get the *error representation*

$$\mathcal{E} := \mathcal{J}(u) - \mathcal{J}(u^h) = (f - L_h u^h, u_* - u_*^h)_Q + O(\|e\|^2)\,.$$

- The error can be estimated as

$$\begin{aligned} |\mathcal{E}| &= |(f - L_h u^h, u_* - u_*^h)_Q| + O(\|e\|^2) \\ &\leq |\mathcal{E}_0| + \sum_{R \in \mathcal{R}} \eta_R + O(\|e\|^2) \qquad \text{for } \eta_R := \rho_R\, \omega_R\,, \end{aligned}$$

  with discretisation error $\mathcal{E}_0$, residuals $\rho_R(u_h)$ and weights $\omega_R(u_* - u_*^h)$.
- The unknown exact dual solution u_* is approximated from the computed solution u_*^h via a polynomial recovery u_*^{rec} of higher order in space and time.

(See e.g. Bangerth and Rannacher 2003)

p and q space-time adaptivity

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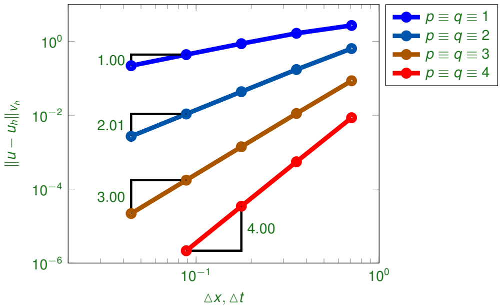
Adaptive Algorithm

- *Compute u^h with lowest polynomial degree $p = 0$ and $q = 1$ on Q*
- *While $p < p_{max}$ and $q < q_{max}$ do:*
  - *Compute the discrete dual solution $\mathbf{u}_*^h$ and a recovery interpolation $\mathbf{u}_*^{rec}$ with degrees $p + 1$ and $q + 1$*
  - *Compute estimated error η_R on a cell $R \in \mathcal{R}$*
  - *Sort the cells descending by η_R and mark e.g. 35% of them for refinement*
  - *Increase the polynomial degrees p_R and q_R on the marked space-time cells $R \in \mathcal{R}$*
  - *Compute $\mathbf{u}^h$ with a new distribution of polynomial degrees*

Performance

- **High** *polynomial degrees are used in areas where it is necessary to* **minimise** $\mathcal{E}$
- **Lowest** *polynomial degrees are used in areas which* **do not effect** $\mathcal{E}$
- *Achieve the* **same accuracy** *as in the global refined case with* **less effort**

Convergence order



Example: EOC for a smooth plane wave solution (acoustic wave).

Solver: GMRES with multigrid preconditioner

- Let $\mathcal{R}_{0,0}$ be a coarse space-time mesh
- Let $\mathcal{R}_{l,k}$ be a fine mesh with $l = 1, \ldots, l_{\max}$ refinements in space and $k = 1, \ldots, k_{\max}$ refinements in time

- Prolongation $P^{l,k}_{l-1,k} \in \mathcal{L}(V_{l-1,k}, V_{l,k})$ (natural injection)
- Restriction $R^{l,k}_{l-1,k} \in \mathcal{L}(W'_{l,k}, W'_{l-1,k})$ (L_2-projection)
- Damped Block-Jacobi smoother $B^{J}_{l,k}$
- Block-Gauss-Seidel smoother $B^{GS}_{l,k}$

Solver: GMRES with multigrid preconditioner

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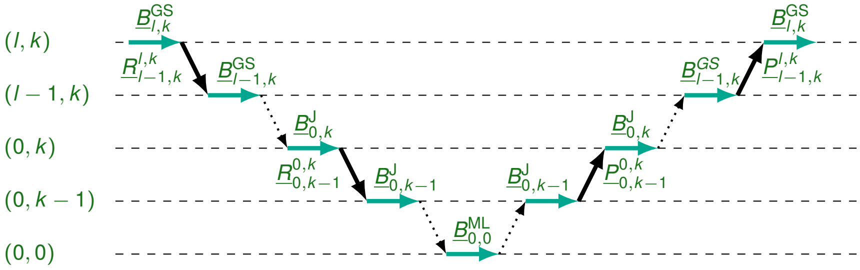

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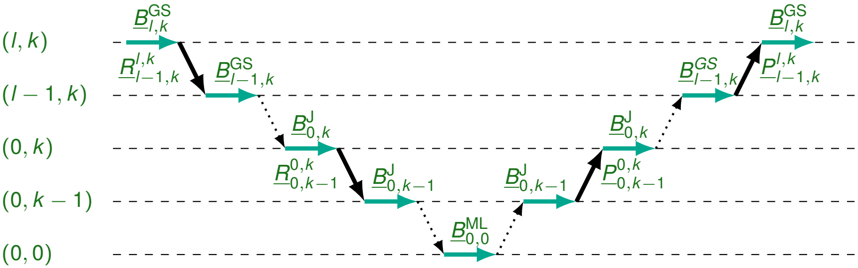

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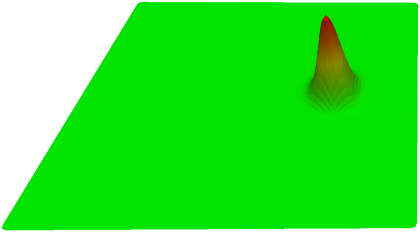
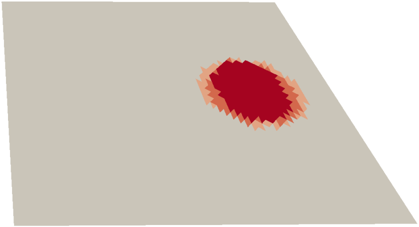
Linear Transport: Rotating Cone (1)

- Initial condition u_0: Gaussian pulse
- Transport vector field: $\boldsymbol{q}(\boldsymbol{x}) = 2\pi[-x_2, x_1]^\dagger$
- DWR: Higher order recovery and $\mathcal{E}(v) = \frac{1}{2}\int_Q |v|^2$



Solution u_h



Distribution of polynomial degrees
(after 4 refinements)

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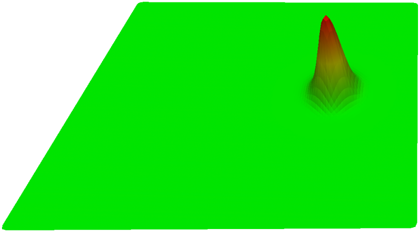

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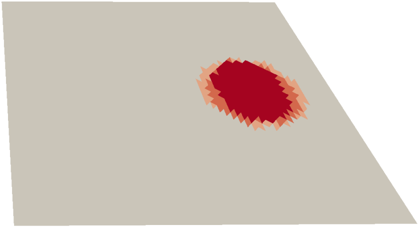

Distribution of polynomial degrees (after 4 refinements)

Numerical Example: Rotating cone (2)

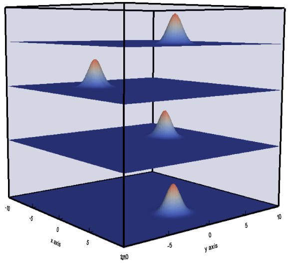

Figure: Solution of the transport equation in the space-time domain Q, sliced at times $t = 0, 0.3, 0.6, 1$.

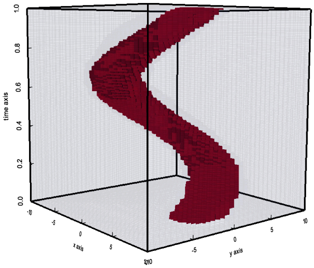

Figure: Location of the highest polynomial degrees in the space-time domain Q.

Numerical Example: Rotating cone (3)

level	uniform poly. deg. (p,q)	#DoFs	GMRES steps (rate)	$\triangle E$	$\|u_h(T)-u(T)\|_\Omega$
$l=1$	(1,1)	1 585 152	10 (7.19e-2)	5.10e-2	4.06e-1
$l=2$	(2,2)	6 340 608	10 (1.30e-1)	2.14e-3	1.97e-2
$l=3$	(3,3)	15 851 520	10 (1.54e-1)	3.78e-5	8.52e-4
$l=4$	(4,4)	31 703 040	11 (1.67e-1)	4.41e-7	5.16e-4

Table: Results for the transport equation with uniform mesh with $524\,288 = 4\,096 \times 128$ space-time cells and different polynomial degrees.

level	#DoFs (effort)	GMRES steps (rate)	$\triangle E$	$\|u_h(T)-u(T)\|_\Omega$	$\|e^*-e_h^*\|_Q$
$l=1$	1 585 152	10 (7.19e-2)	5.10e-2	4.06e-1	1.78e-1
$l=2$	1 894 176 (30%)	10 (9.53e-2)	2.14e-3	2.02e-2	9.98e-3
$l=3$	2 381 598 (15%)	10 (1.43e-1)	3.79e-5	1.87e-3	8.40e-4
$l=4$	3 303 810 (10%)	11 (1.23e-1)	4.31e-7	5.22e-4	5.29e-4

Table: Adaptive refinement on a mesh with $524\,288 = 4\,096 \times 128$ space-time cells ($\vartheta = 1\text{e-}4$).

Numerical Example: Travelling Wave (1)

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Solution of the wave equation (special case of Maxwell's equation).

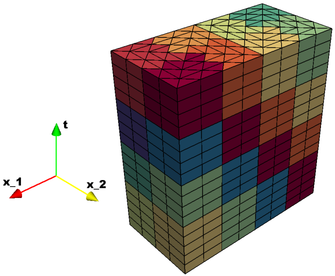
We consider

- a wave $\boldsymbol{u}(t,\boldsymbol{x}) = \boldsymbol{a}(\boldsymbol{x}\cdot\boldsymbol{k} - ct)$ with an amplitude profile

$$\boldsymbol{a}(z) = \left(\cos(2\pi(z-\frac{1}{2}))+1\right)^2 [0,-1,1]^T$$

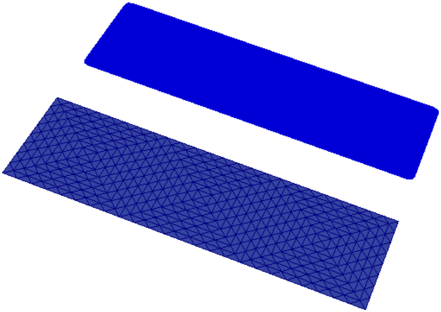
  in $Q = (0,3)\times(0.5,0.5)\times(0,T)$ with final time $T=4$ and Dirichlet boundary conditions,
- constant material parameters $\mu = \varepsilon = 1$,
- the energy error functional

$$\mathcal{E}(\boldsymbol{e}) := \frac{1}{2}(M\boldsymbol{e},\boldsymbol{e})_Q\,.$$



Distribution of space-time cells on 32 processes

Numerical Example: Travelling Wave (2)



Back: Time evolution of a travelling wave
Front: Used polynomial degrees

Numerical Example: Travelling Wave (3)

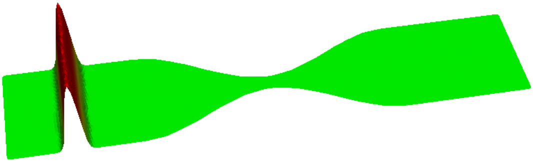
Adaptive refinement with $p_\tau \in \{0, 1, 2, 3\}$ in space and $q_\tau \in \{1, 2, 3, 4\}$ in time.

p, q-level	adaptive #DoFs	adaptive $\|\mathcal{E}(\boldsymbol{e})\|$	uniform #DoFs	uniform $\|\mathcal{E}(\boldsymbol{e})\|$
0	149 760	4.51e-0	149 760	4.51e-0
1	437 955	1.65e-1	898 560	1.65e-1
2	1 104 297	1.75e-3	2 695 680	1.83e-3
3	2 277 720	5.20e-5	5 990 400	1.43e-5

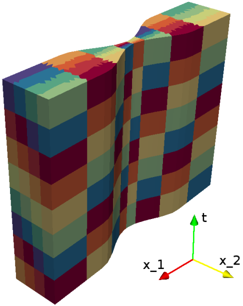
Space-time adaptive refinement and corresponding degrees of freedom.

By using adaptivity we achieve nearly the same accuracy as in the globally refined case with approximately 38% degrees of freedom on the finest level.

Numerical Example: Tapered domain



Time evolution of a wave in a tapered domain – the problem was solved in about 12 min on 256 processes (with about 30 mio degrees of freedom) and about 25 min on 1024 processes (with about 180 mio degrees of freedom). Reduction to 27%, reps. 21% of the unknowns.



Distribution of space-time cells on 256 processes.

Numerical Example: Double-slit (1)

We consider

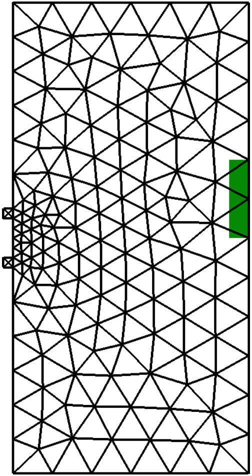
- an interfering wave in a double-slit experiment with reflecting boundary conditions,
- constant material parameters $\mu = \varepsilon = 1$, wavelength $\lambda = 0.5$, slit gap $a = 1.25$ and slit width $b = 0.25$,
- the linear error functional

$$\mathcal{J}(\boldsymbol{e}) := |S|^{-1} \int_S \boldsymbol{e}_y \, \mathrm{d}(x,t)$$

  with region of interest
  $S := (5.5, 6) \times (0, 2) \times (0, 8)$
  (e.g. photosensitive detector),
- known diffraction pattern for the far field

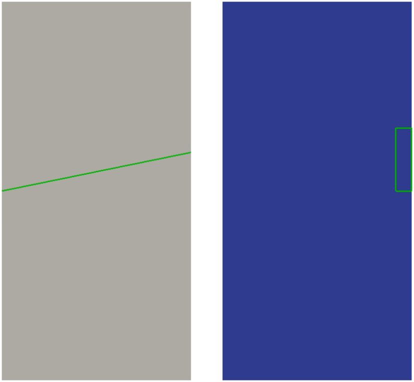
$$I_{\text{diff}}(\alpha) = I_0 \operatorname{sinc}^2\left(\frac{\pi}{\lambda} b \sin\alpha\right) \cos^2\left(\frac{\pi}{\lambda} a \sin\alpha\right)$$

  in dependence of the observation angle α.



Triangular mesh in domain Ω with region of interest S on level $l = 0$.

Numerical Example: Double-slit (2)



Left: Time evolution of an interfering wave and the location of a theoretical minimum.

Right: Used polynomial degrees and region of interest.

Visco-Elastic Wave inspired by Marmousi I

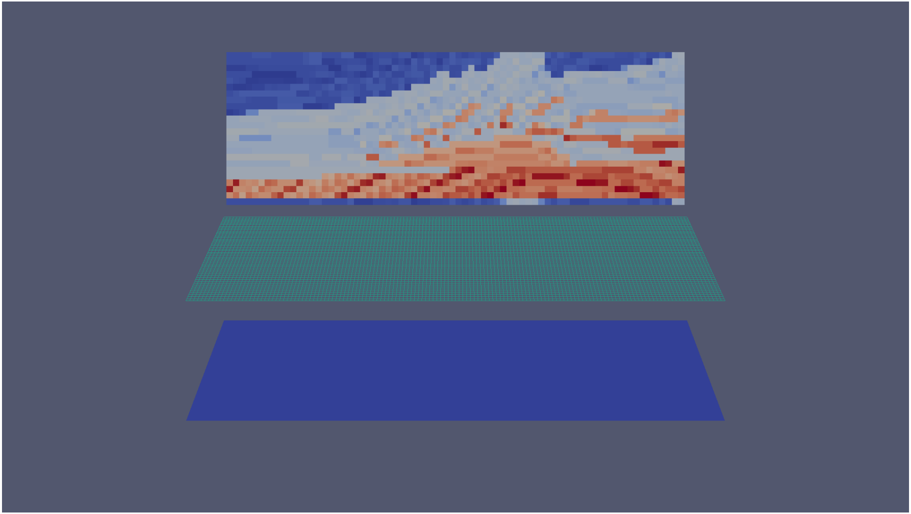
Visco-elastic waves, application from Geophysics

$$\rho\,\partial_t \vec{v} = \nabla \cdot \vec{\sigma}_0 + \cdots + \nabla \cdot \vec{\sigma}_L + \vec{f}\,,$$
$$\partial_t \vec{\sigma}_0 = \vec{C}_0 \vec{\varepsilon}(\vec{v})\,,$$
$$\partial_t \vec{\sigma}_l = \vec{C}_l \vec{\varepsilon}(\vec{v}) - \frac{1}{\tau_l}\vec{\sigma}_l\,, \qquad l = 1, \ldots, L\,.$$

Latest results:

- starting with linear functions making one adaptive step
- Problem size: 442 859 696 of 1 019 215 872
- 24 GMRES steps using MG-preconditioner in less than 15 min
- computed using 8192 cores

Visco-Elastic Wave inspired by Marmousi I



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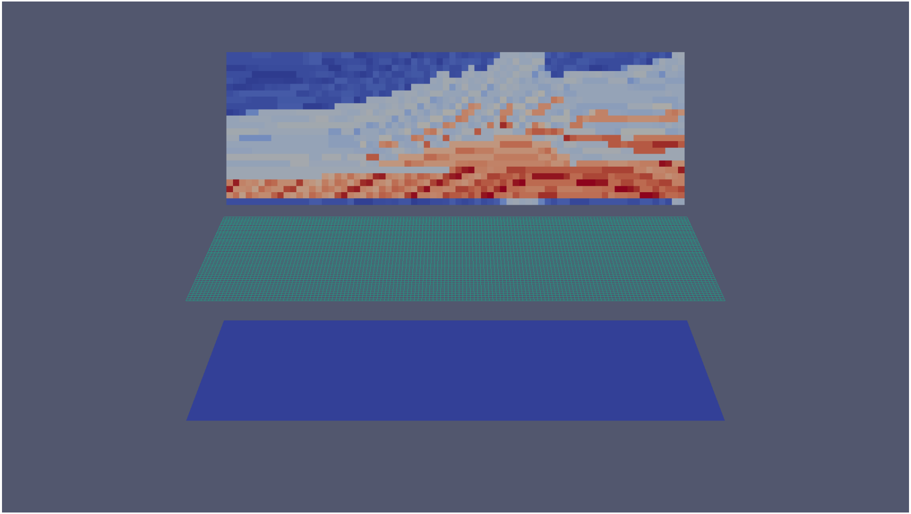

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