Discontinuous Galerkin Space-Time Finite Element method for two-phase mass transport

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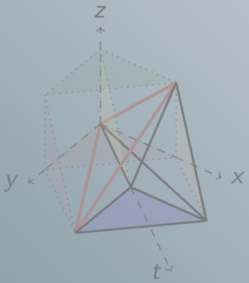
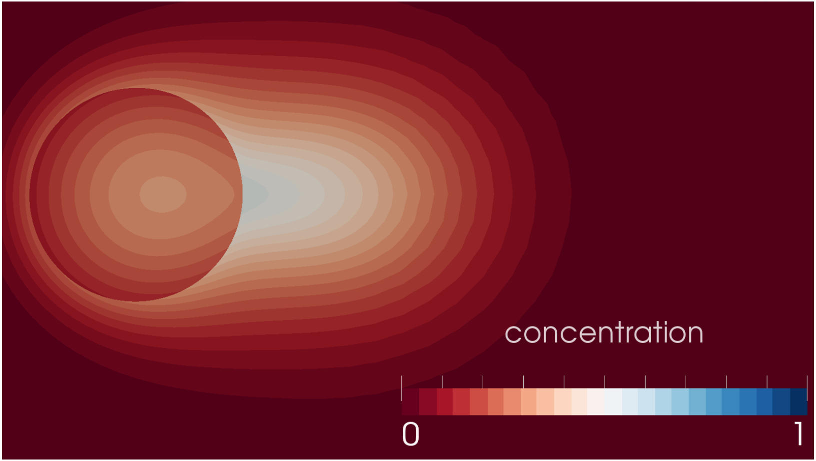
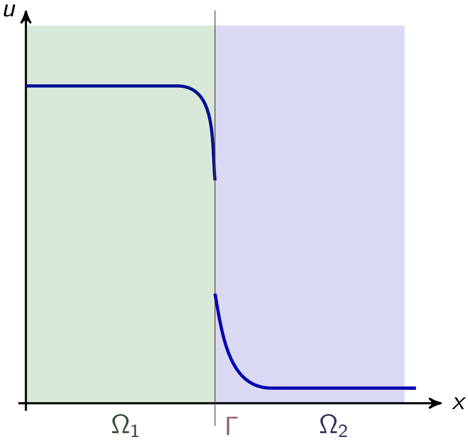


Two-phase mass transport: A movie



Situation at the interface



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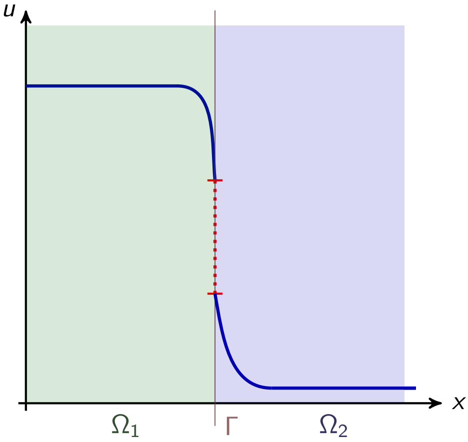
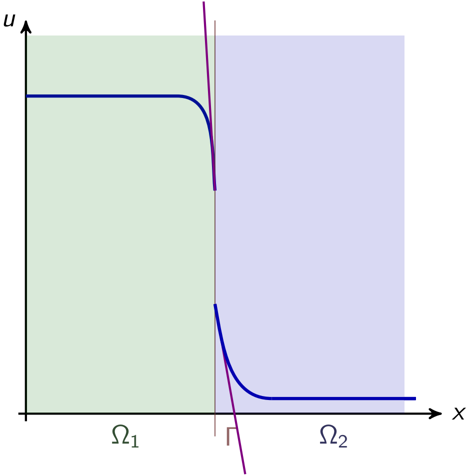


discontinuous conc.
$u_1/u_2 = \beta_2/\beta_1$

Situation at the interface



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disc. normal derivative
$\alpha_1 \frac{\partial u_1}{\partial \mathbf{n}_1} = \alpha_2 \frac{\partial u_2}{\partial \mathbf{n}_2}$

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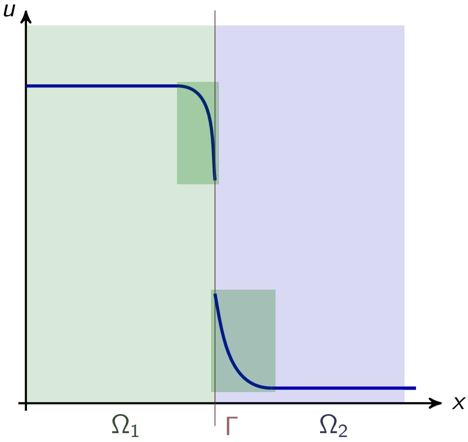

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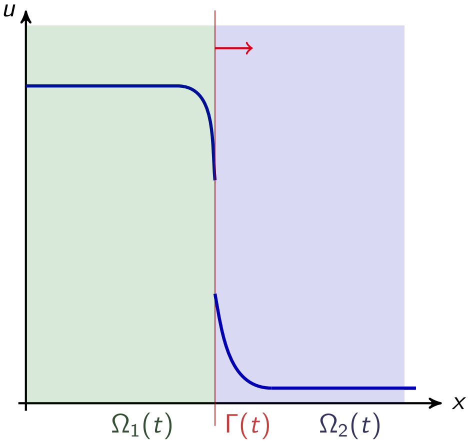
sharp layers

Situation at the interface



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disc. normal derivative
$\alpha_1 \frac{\partial u_1}{\partial \mathbf{n}_1} = \alpha_2 \frac{\partial u_2}{\partial \mathbf{n}_2}$

sharp layers

moving interface $\Gamma(t)$

Mass transport

Mass transport equation

$$\frac{\partial u}{\partial t} + \mathbf{w} \cdot \nabla u - \alpha \Delta u = 0 \qquad \text{in } \Omega_1 \cup \Omega_2,$$

$$[\![-\alpha \nabla u]\!] \cdot \mathbf{n} = 0 \qquad \text{on } \Gamma,$$

$$[\![\beta u]\!] = 0 \qquad \text{on } \Gamma.$$

$$\mathcal{V} \cdot \mathbf{n} = \mathbf{w} \cdot \mathbf{n} \quad \text{on } \Gamma.$$

$$\mathrm{div}(\mathbf{w}) = 0 \qquad \text{in } \Omega$$

u: concentration,
α: piecewise constant diffusion coefficients,
β: piecewise constant Henry coefficients,
$\mathbf{w}$: convection velocity (from Navier Stokes)
$\mathcal{V}$: the interface velocity
Henry condition: discontinuity in u.

Numerical Aspects

Mass transport equation

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Numerical Challenges

- Level set to capture the interface
  $\Rightarrow$ Interface is not aligned with the mesh (might depend on time)
- concentration has discontinuities (approximation)
- time integration for (non-matched) moving interfaces
- problem is typically highly convection dominated (stability)

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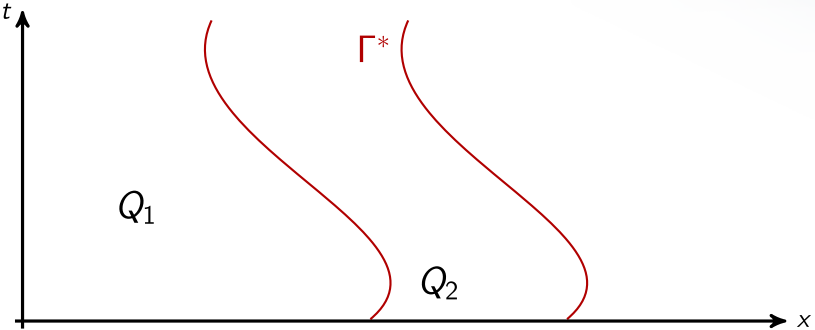
Numerical Approaches

- Space-time formulation on each time slab
- Extended Finite Element space (XFEM)
- Nitsche-type technique to enforce Henry's law in a weak sense
- (Space-time Streamline Diffusion) Stabilization

Space-time weak formulation I



Anisotropic Spaces; $Q = Q_1 \cup Q_2$

$$V_\beta = \left\{ u \in L^2(Q) \mid u_i \in H^{1,0}(Q_i),\ i = 1, 2,\ u_{|\partial\Omega} = 0,\ [\![\beta u]\!]_{\Gamma_*} = 0 \right\}$$

$$W_\beta = \left\{ v \in V_\beta \mid \frac{\partial v}{\partial t} \in H_0^{1,0}(Q)' \right\}.$$

Space-time weak formulation II

Well-posed weak formulation [Gross/Reusken 11]

Determine $u \in W_\beta$ with $u(\cdot, 0) = 0$ such that

$$\frac{\partial u}{\partial t}(v) - \int_Q u\mathbf{w} \cdot \nabla v \, dx \, dt + \sum_{i=1}^{2} \int_{Q_i} \alpha_i \nabla u_i \cdot \nabla v \, dx \, dt = \int_Q fv \, dx \, dt$$

for all $v \in H_0^{1,0}(Q) \neq V_\beta$

Remarks:

- Space-time (n+1 dimensional) formulation
- Trial functions are discontinuous across Γ_*
- Condition $[\![\beta u]\!]_\Gamma = 0$ essential condition in space W_β

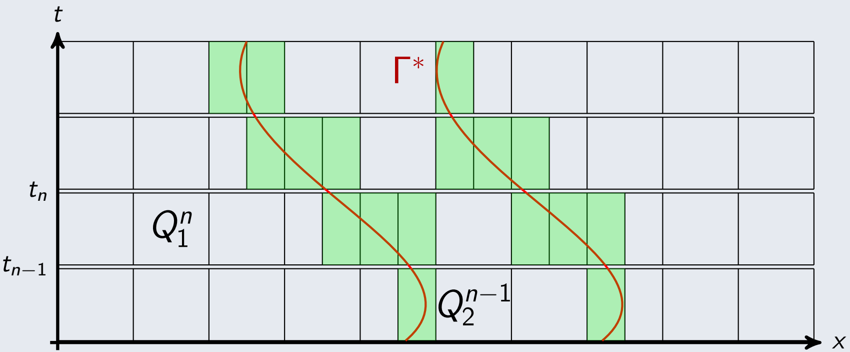
Nitsche-DG-XFEM discretization

Space-time FE

$I_n = (t_{n-1}, t_n]$, $Q^n = \Omega \times I_n$. V_n : standard FE space on Ω.

$$W_n := \{\, v : Q^n \to \mathbb{R} \mid v(x,t) = \phi_0(x) + t\phi_1(x), \quad \phi_0, \phi_1 \in V_n \,\}$$

$$W := \{\, v : Q \to \mathbb{R} \mid v_{|Q^n} \in W_n \,\} \quad \text{(space-time FE).}$$

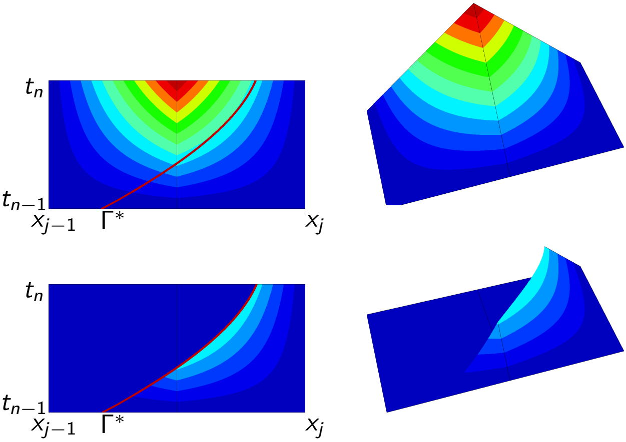


Approximating discontinuities

Space-time FE $\Rightarrow$ Space-time XFEM

$$Q_i^n := \cup_{t \in I_n} \Omega_i(t), \quad R_i^n: \quad \text{restriction to } Q_i^n$$

$$W_n^\Gamma := R_1^n W_n \oplus R_2^n W_n, \quad W^{\Gamma *} := \{\, v : Q \to \mathbb{R} \mid v_{|Q^n} \in W_n^\Gamma \,\}$$



Bilinear forms (within time slab Q^n) I

Conforming part

$$a^n(u, v) = \sum_{i=1}^{2} \int_{Q_i^n} \Big(\frac{\partial u_i}{\partial t} + \mathbf{w} \cdot \nabla u_i\Big)\beta_i v_i + \alpha_i \beta_i \nabla u_i \cdot \nabla v_i \, dx \, dt$$

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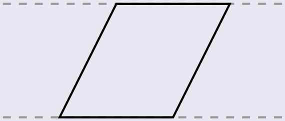
Discontinuous Galerkin Upwind w.r.t. time:

$$d^n(u,v) = \int_{\Omega} \beta(\cdot, t_n)[u]^{n-1} v_+^{n-1}\, dt$$

Bilinear forms (within time slab Q^n) II

Nitsche method for Henry condition:

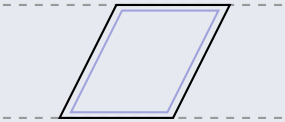
$$-\int_{Q^n} \beta \mathrm{div}(\alpha \nabla u) v \, dx$$



Bilinear forms (within time slab Q^n) II

Nitsche method for Henry condition:

$$-\int_{Q^n} \beta \operatorname{div}(\alpha \nabla u) v \, dx = \int_{Q^n} \alpha \beta \nabla u \nabla v \, dx - \int_{\partial Q^n} \begin{pmatrix} \alpha \nabla u \\ 0 \end{pmatrix} \cdot (\mathbf{n}^*) \, v \, ds$$

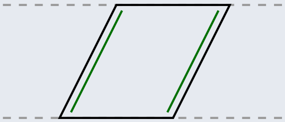


Bilinear forms (within time slab Q^n) II

Nitsche method for Henry condition:

$$-\int_{Q^n} \beta \mathrm{div}(\alpha \nabla u) v \, dx = \int_{Q^n} \alpha\beta \nabla u \nabla v \, dx - \int_{\partial Q^n} \begin{pmatrix} \alpha \nabla u \\ 0 \end{pmatrix} \cdot (\mathbf{n}^*) \, v \, ds$$

$$= \quad \ldots - \int_{\Gamma_*^n} \nu \alpha \nabla u \cdot \mathbf{n} \beta v \, ds$$



$\nu = 1/\sqrt{1 + (\mathbf{w} \cdot \mathbf{n})^2}$: $\int_{t^{n-1}}^{t^n} \int_{\Gamma^n} f \, ds \, dt = \int_{\Gamma_*^n} \nu f \, ds$,

Bilinear forms (within time slab Q^n) II

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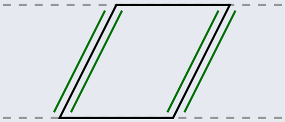
$$\rightarrow \quad \ldots - \sum_{i=1}^{2} \int_{\Gamma_*^n} \nu \{\alpha \nabla u \cdot \mathbf{n}\}_{\Gamma_*^n} \beta_i v \, ds$$

$$= \quad \ldots - \int_{\Gamma_*^n} \nu \{\alpha \nabla u \cdot \mathbf{n}\}_{\Gamma_*^n} [\beta v]_{\Gamma_*^n} \, ds$$

A



with $\{\cdot\}_{\Gamma_*^n}$ suitable volume weighted average.

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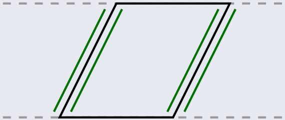

$$\longrightarrow \quad - \int_{\Gamma_*^n} \nu \{\alpha \nabla v \cdot \mathbf{n}\}_{\Gamma_*^n} [\beta u]_{\Gamma_*^n} \, ds \quad \text{(B)} \quad + \lambda h_n^{-1} \int_{\Gamma_*^n} \nu [\beta u]_{\Gamma_*^n} [\beta v]_{\Gamma_*^n} \, ds, \quad \text{(C)}$$

with $\{\cdot\}_{\Gamma_*^n}$ suitable volume weighted average. $\lambda > 0$: stabilization parameter

and $\nu = 1/\sqrt{1 + (\mathbf{w} \cdot \mathbf{n})^2}$: $\int_{t^{n-1}}^{t^n} \int_{\Gamma^n} f \, ds \, dt = \int_{\Gamma_*^n} \nu f \, ds$,

$$N_{\Gamma_*}^n(c, v) := \text{(A)} + \text{(B)} + \text{(C)}$$

Nitsche-DG-XFEM variational problem

global bilinearforms

$$a(u,v) = \sum_{n=1}^{N} a^n(u,v), \quad \text{similarly :} \quad d(u,v),\ N_{\Gamma_*}(u,v).$$

Discrete problem

Determine $U \in W^{\Gamma_*}$ such that

$$B(U,V) = f(V) \quad \text{for all} \quad V \in W^{\Gamma_*},$$
$$B(U,V) := a(U,V) + d(U,V) + N_{\Gamma_*}(U,V).$$

Error analysis (results)

Theorem

Error analysis for linear (space+time) FE

$$\|(u-U)(\cdot,t_N)\|_{L^2(\Omega^N)} \leq c(h^2+\Delta t^2).$$

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$$\|(u - U)(\cdot, t_N)\|_{L^2(\Omega^N)} \leq c(h^2 + \Delta t^2).$$

Remark:

for standard space-time DG [V. Thomee] (no Nitsche, no XFEM):

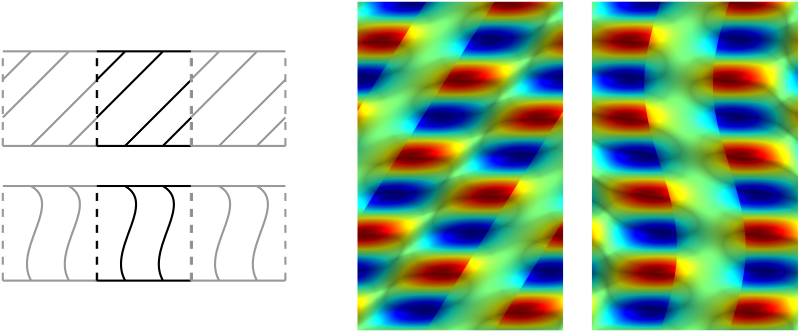
$$\|(u - U)(\cdot, t_N)\|_{L^2(\Omega^N)} \leq c(h^2 + \Delta t^3)$$

Concept of V. Thomee needs tensor product decomposition of the spaces which we don't have for moving interfaces.

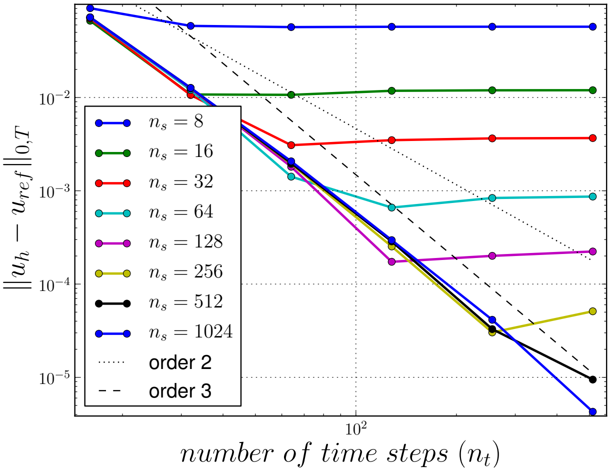
Numerical experiment

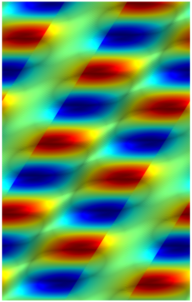
Numerical example in (1+1)D

Diffusion dominates, periodic boundary conditions, artificial source terms



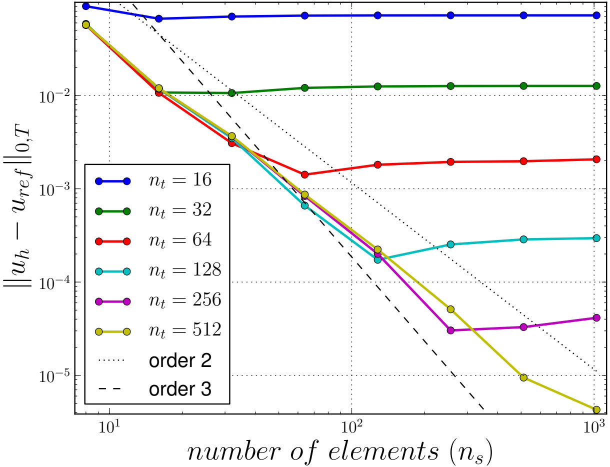
Discretization error (temporal convergence)

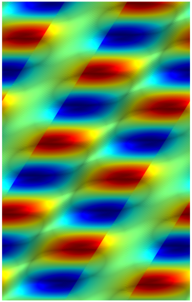




This indicates: $\|(U-u)(\cdot, t_N)\|_{L^2(\Omega)} \sim \Delta t^3$ **if** h **sufficiently small.**

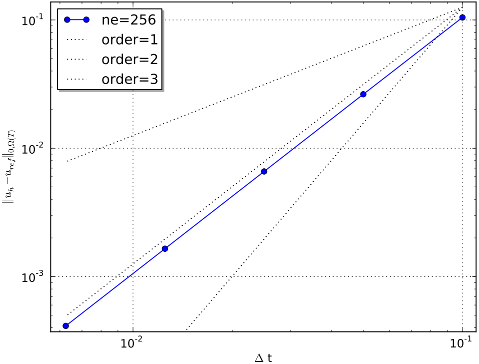
Discretization error (spatial convergence)

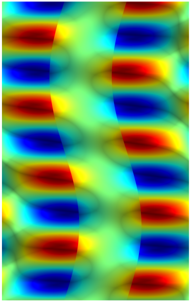




This indicates: $\|(U-u)(\cdot, t_N)\|_{L^2(\Omega)} \sim h^2$ if Δt sufficiently small.

Numerical example (continued): Non-planar interface





This indicates: $\|(U-u)(\cdot,t_N)\|_{L^2(\Omega)} \sim$ ~~Δt^3~~ Δt^2 if h sufficiently small.

With sufficiently fine quadrature we reobtain $\|(U-u)(\cdot,t_N)\|_{L^2(\Omega)} \sim \Delta t^3$.

Conclusion

Discretization

- (Domain-)piecewise continuous approximation + XFEM
- Nitsche(-XFEM) for interface conditions
- Space-time FEM with (P1) Discontinuous Galerkin in time.
  [**space-time integrals** ⇒ *Composite quadrature in (n+1) D*]

Quadrature in (3+1)D

- Quadr. on cutted 4D geometries ⇒ **decomposition** rules **into pentatopes**
- Implementation on the way
- Limitations (so far?!) to planar space-time interfaces ⇒ $\mathcal{O}(\Delta t^2)$

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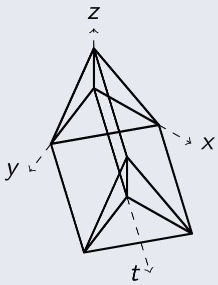
Thank you for your attention!

Decomposition into simplices

The reference element can be decomposed into simplices

$(1+1):$ $\hat{Q}$ is a square $\rightarrow$ 2 triangles
$(2+1):$ $\hat{Q}$ is a (regular) prism $\rightarrow$ 3 tetrahedra
$(3+1):$ $\hat{Q}$ is a (regular) prism-4 $\rightarrow$ 4(?) pentatopes(?)

The reference prism-4 $\hat{Q}$



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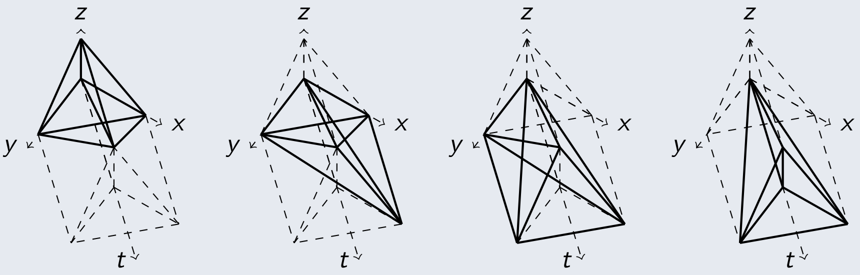
$$

The reference prism-4 $\hat{Q}$ and it's decomposition



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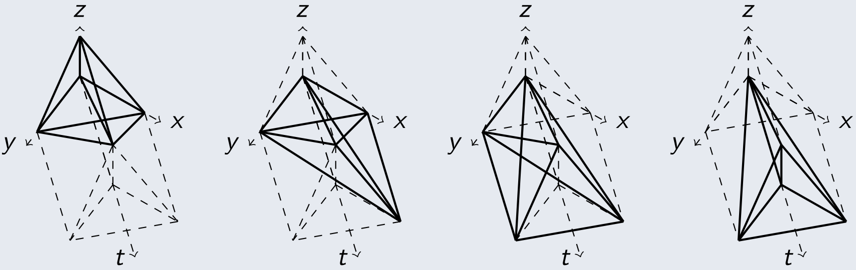
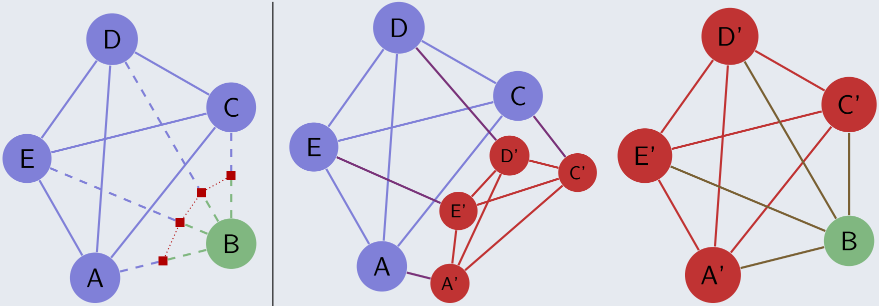


Consider the quadrature problem on (n+1)-simplex!

Slicing the pentatope

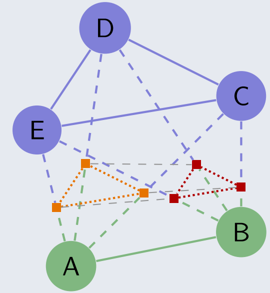
(Non-degenerated) Case 1:

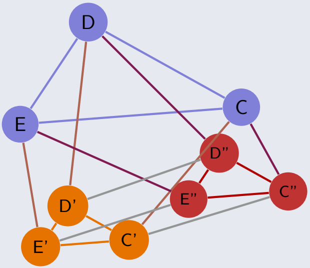


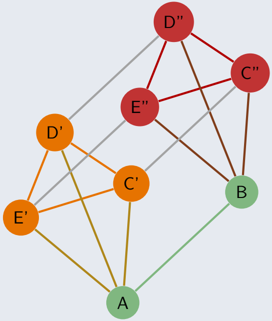
cutted pentatope	(irregular) prism-4	+	pentatope
	↓ (decomposition)		↓
	4 pentatopes	+	1 pentatope
interface	1 tetrahedra		

Slicing the pentatope

(Non-degenerated) Case 2:



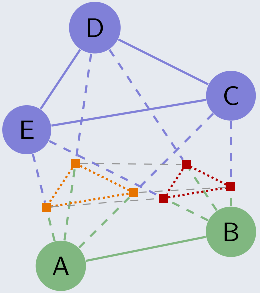


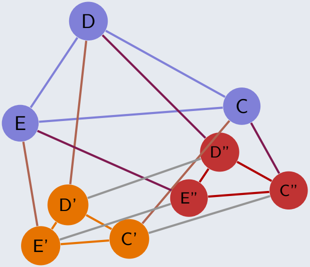


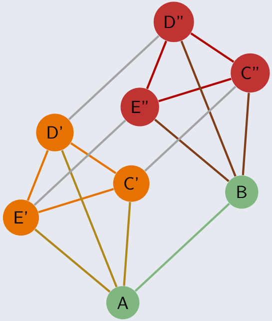
cutted pentatope	(irregular) hypertriangle ↓ (decomposition) 6 pentatopes	+ (irregular) prism-4 ↓ + 4 pentatopes
interface	prism-3 → 3 tetrahedra	

Slicing the pentatope

(Non-degenerated) Case 2:





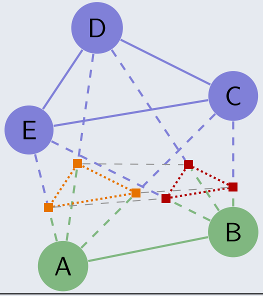


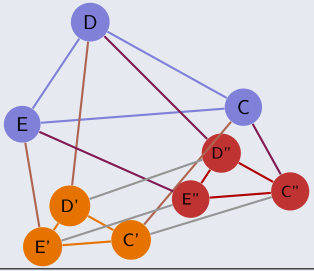
cutted pentatope	(irregular) hypertriangle ↓ (decomposition) 6 pentatopes	+ +	(irregular) prism-4 ↓ 4 pentatopes
interface	prism-3 → 3 tetrahedra		

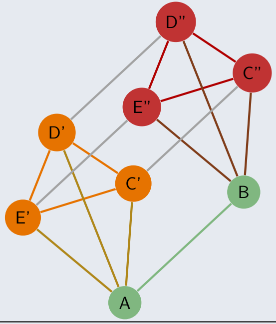
Step 4: Decomposition into one-phase (n+1)-simplices and n-simplices!

Slicing the pentatope

(Non-degenerated) Case 2:







cutted pentatope	(irregular) hypertriangle	+	(irregular) prism-4
	↓ (decomposition)		↓
	6 pentatopes	+	4 pentatopes
interface	prism-3 → 3 tetrahedra		

Step 4: Decomposition into one-phase (n+1)-simplices and n-simplices!

Decomposition of the hypertriangle into 6 pentatopes