Numerical Methods for Two-Phase Flows with Mass Transport

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Introduction

Problem classes



- Fluid dynamics for Two-Phase (immiscible) incompressible flows: (Navier-Stokes Eqns. + surface tension effects)
- with mass transport (convection-diffusion eqn. + Henry interface condition)
- and surfactant transport (convection-diffusion eqn. on the surface)

applications:

- falling film (gas-liquid)
- rising bubble (liquid-liquid)
- taylor flow (gas-liquid)



Processes at (close to) the interface!

Standard (sharp interface) model for Two-Phase flows

Domains: $\Omega_1 = \Omega_1(t)$ and $\Omega_2 = \Omega_2(t)$

Interface: $\Gamma = \Gamma(t) = \partial \Omega_1 \cap \partial \Omega_2$

 $\begin{array}{ll} \rho_i: & \mbox{density in } \Omega_i \\ \mu_i: & \mbox{viscosity in } \Omega_i \\ \tau: & \mbox{surface tension coefficient} \\ \mathbf{D}(\mathbf{w}) = \nabla \mathbf{w} + \nabla \mathbf{w}^T, \ \sigma = -p \ \mathbf{I} + \mu \mathbf{D}(\mathbf{w}) \\ \kappa: & \mbox{curvature} \end{array}$



Navier-Stokes equations

$$\begin{cases} \rho_i \big(\mathbf{w}_t + (\mathbf{w} \cdot \nabla) \mathbf{w} \big) = \operatorname{div} (\sigma) + \rho_i \mathbf{g} & \text{in } \Omega_i \\ \\ \operatorname{div} \mathbf{w} = 0 & \text{in } \Omega_i \end{cases} \quad \text{for } i = 1, 2 \end{cases}$$

$$\llbracket \sigma \mathbf{n} \rrbracket_{\Gamma} = \tau \kappa \mathbf{n} + \nabla_{\Gamma} \tau, \quad \llbracket \mathbf{w} \rrbracket_{\Gamma} = \mathbf{0} \;.$$

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$$\llbracket \sigma \mathbf{n} \rrbracket_{\Gamma} = \tau \kappa \mathbf{n} + \nabla_{\Gamma} \tau, \quad \llbracket \mathbf{w} \rrbracket_{\Gamma} = \mathbf{0} .$$

How to identify the interface?

Interface capturing: Level set approach



the level set function $\varphi(x, t)$

$$\varphi(x,t) = \begin{cases} < 0 & \text{for } x \text{ in phase } \Omega_1 \\ > 0 & \text{for } x \text{ in phase } \Omega_2 \\ = 0 & \text{at the interface} \end{cases}$$



should be an "approximate signed distance function". $x(t) \in \Gamma(t) \Rightarrow \varphi(x(t), t) = 0.$

Level set equation

$$\varphi_t + \mathbf{w} \cdot \nabla \varphi = 0$$
 in Ω

Level set approach: Pros and Cons

Eulerian vs. Lagrangian

Level set description allows us to stay in a purely Eulerian framework.

Interface capturing (in contrast to interface tracking (e.g. ALE))

- + no remeshing
- + topology changes (breakups, coalescence) and large deformations
- interface description implicitely (interface is not meshed)
- tracking of evolution of particles at or close to interface

Level set (in contrast to VOF)

- + accuracy of (implicit) interface
- no discrete mass conservation
- (+) signed distance property
- signed distance property gets lost (re-initialization)

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Level set (in contrast to VOF)

- + accuracy of (implicit) interface
- no discrete mass conservation (videos, JB)
- (+) signed distance property
- signed distance property gets lost (re-initialization)

- no corr. (1 b.),
- single corr. (1 b.)
- single corr. (2 b.)
- multicomp. corr. (2 b.)

Model: Navier-Stokes + level set equation

Navier-Stokes equations coupled with level set equation ($\tau = const$)

$$\rho(\varphi) \Big(\mathbf{w}_t + (\mathbf{w} \cdot \nabla) \mathbf{w} \Big) - \operatorname{div} \Big(\mu(\varphi) \, \mathbf{D}(\mathbf{w}) \Big) + \nabla p = \rho(\varphi) \, g - \tau \, \kappa(\varphi) \, \delta_{\Gamma} \mathbf{n}_{\Gamma} \\ \operatorname{div} \mathbf{w} = \mathbf{0}$$

$$\varphi_t + \mathbf{w} \cdot \nabla \varphi = 0$$

where ρ, μ and $\kappa, \delta_{\Gamma}, \mathbf{n}_{\Gamma}$ depend on φ .

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$$\varphi_t + \mathbf{w} \cdot \nabla \varphi = 0$$

where ρ, μ and $\kappa, \delta_{\Gamma}, \mathbf{n}_{\Gamma}$ depend on φ .

Additional equations

Surfactant transport (on the interface):

$$s_t + \mathbf{w} \cdot \nabla_{\Gamma} s - \mu_{\Gamma} \Delta_{\Gamma} s = f_{\Gamma} \quad \text{on } \Gamma$$

Mass transport (discontinuity across the interface):

$$\begin{aligned} u_t + \mathbf{w} \cdot \nabla u - \alpha \Delta u &= f & \text{in } \Omega_i \\ \llbracket \alpha \frac{\partial u}{\partial \mathbf{n}} \rrbracket = \mathbf{0}, \quad \llbracket \beta u \rrbracket = \mathbf{0} & \text{on } \Gamma \end{aligned}$$

Interface capturing with Level-Set

Discretization background



Starting point

- \blacktriangleright Adaptive tetrahedral mesh for $\Omega=\Omega_1\cup\Omega_2$
- Conforming finite elements:
 - P2-P1 Taylor-Hood elements (continuous)
 - P2 for level set (continuous)
 - P1 for mass/surfactants transport (continuous)
- Method of lines time integration (implicit euler, etc..)

Numerical Challenges

Key problems

- Multiscale phenomena close to the interface.
- Highly nonlinear couplings between **w**, φ , f_{Γ} , c, c_{Γ} .
- Interesting modeling aspects, e.g.: $\tau = \tau(c, c_{\Gamma})$ (YZ) or coalescence (JB)
- Accurate resolution of unknown interface.
 Treatment of the level set equation (EL), volume correction (JB)
- Treatment of surface tension force (Laplace-Beltrami discretization)
- Treatment of discontinuous pressure
- Treatment of kinks in velocity (SG)
- Coupling of flow + interface dynamics + transport equations.
- Discretization of transport equation with (moving) discontinuities (CL)
- ▶ Discretization of transport equation on (moving) interface (JG) + (XZ)
- Efficiency/robustness of iterative solvers.
- High complexity: parallel solvers needed, (SG) + (PE)
- Higher order time integration (space-time formulation) (PE)

Interface force balance



Interface condition

We have the condition:

$$\llbracket \sigma \mathbf{n} \rrbracket_{\Gamma} = \llbracket (\mu D(\mathbf{w}) + \rho I) \mathbf{n} \rrbracket_{\Gamma} = \tau \kappa \mathbf{n} \ (+\nabla_{\Gamma} \tau)$$

Typically:

Non-aligned mesh + standard polynomial FE space Q_h \Rightarrow approximation quality reduces to

$$\inf_{p_h \in Q_h} \|p - p_h\|_{L^2} \leq \mathcal{O}(\sqrt{h})$$

Handling Discontinuities: Domain-wise cont. ansatz $Q_h^{\Gamma} := Q_h(\tilde{\Omega_1}) \cdot H^{\Gamma} \oplus Q_h(\tilde{\Omega_2}) \cdot (1 - H^{\Gamma})$



Handling Discontinuities: Add. ansatz functions (XFEM)

Remedy

and

Extend P_1 FE basis with discontinuous basis functions near Γ :

$$p_j^{\Gamma} := p_j \ (H_{\Gamma}(x) - H_{\Gamma}(x_j)), \quad H_{\Gamma} = \begin{cases} 1 & \text{in } \Omega_1 \\ 0 & \text{in } \Omega_2 \end{cases}$$
use $Q_h^{\Gamma} = Q_h \oplus \{p_j^{\Gamma}\}$





Two-Phase Hydrodynamic Numerical Challenges

Handling (Pressure) Discontinuities: XFEM

Remarks

- ▶ In practice: Γ_h instead of Γ .
- $\dim(Q_h^{\Gamma})$ depends on Γ .
- New basis functions can have very small supports.
- other applications: [Belytschko (1999 ->)]: elasticity, [Hansbo (2002 ->)]: interf. probl., Two-Phase Mass Transport



P2-P1-Taylor-Hood + XFEM for pressure

Enrichment: we use a P1X finite element space for the pressure space.

- (+) pressure approximation is optimal: $\mathcal{O}(h^2)$ in L^2 -norm.
- () no LBB-stability result for velocity-pressure pair ($V_h, Q_h^{\Gamma})$ any more

Kinks in velocity field also need a "kink-version" XFEM!

Key components in DROPS:

- Hybrid level set technique for interface capturing
- Adaptive multilevel triangulations (tetrahedra) + Finite Elements (not aligned to the interface)
- Special quadrature techniques (discontinuous μ, ρ)
- ▶ Discretization of localized force term f_{Γ} : Laplace-Beltrami
- ► Finite element space for discontinuous pressure: XFEM
- Special iterative solvers: robustness w.r.t. h, Δt , jumps in ρ , (μ)
- MPI based parallelization (Institute for Scientific Computing)
- Surfactant transport equation: Interface FE method
- Mass transport equation: Nitsche-XFEM method

Numerical Challenges

Some DROPS movies





Two-Phase Mass Transport Mass Transport Problem statement

Two-Phase mass transport: A movie

























Mass transport

Mass transport equation

$$\begin{split} \frac{\partial u}{\partial t} + \, \mathbf{w} \cdot \nabla u - \alpha \Delta u &= 0 \qquad \text{ in } \Omega_1 \cup \Omega_2, \\ \left[\!\left[-\alpha \nabla u \right]\!\right] \cdot \mathbf{n} &= 0 \qquad \text{ on } \Gamma, \\ \left[\!\left[\beta u \right]\!\right] &= 0 \qquad \text{ on } \Gamma. \end{split}$$

$$\mathcal{V} \cdot \mathbf{n} = \mathbf{w} \cdot \mathbf{n}$$
 on Γ .
div $(\mathbf{w}) = 0$ in Ω

u: concentration,

- α : piecewise constant diffusion coefficients,
- β : piecewise constant Henry coefficients,
- w: convection velocity (from Navier Stokes)
- $\mathcal{V}:$ the interface velocity

Henry condition: discontinuity in *u*.

Numerical Aspects

Mass transport equation

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

$$\begin{bmatrix} -\alpha \nabla u \end{bmatrix} \cdot \mathbf{n} = 0 \quad \text{on } \Gamma(t),$$

$$\begin{bmatrix} \beta u \end{bmatrix} = 0 \quad \text{on } \Gamma(t).$$

Numerical Aspects

Mass transport equation

$$\begin{aligned} \frac{\partial u}{\partial t} + \mathbf{w} \cdot \nabla u - \alpha \Delta u &= 0 \quad \text{ in } \Omega_1(t) \cup \Omega_2(t), \\ \begin{bmatrix} -\alpha \nabla u \end{bmatrix} \cdot \mathbf{n} &= 0 \quad \text{ on } \Gamma(t), \\ \begin{bmatrix} \beta u \end{bmatrix} &= 0 \quad \text{ on } \Gamma(t). \end{aligned}$$

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)

Numerical Aspects

Numerical Challenges

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Numerical Approaches

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



Space-time weak formulation I



Anisotropic Spaces; $Q = Q_1 \cup Q_2$

$$V_{\beta} = \{ u \in L^{2}(Q) \mid u_{i} \in H^{1,0}(Q_{i}), i = 1, 2, u_{|\partial\Omega} = 0, [[\beta u]]_{\Gamma_{*}} = 0 \}$$
$$W_{\beta} = \{ v \in V_{\beta} \mid \frac{\partial v}{\partial t} \in H^{1,0}_{0}(Q)' \}.$$

Space-time weak formulation II



Well-posed weak formulation [Gross/Reusken 11]

Determine $u \in W_{eta}$ with $u(\cdot, 0) = 0$ such that

$$\frac{\partial u}{\partial t}(v) - \int_{Q} u \mathbf{w} \cdot \nabla v \, dx \, dt + \sum_{i=1}^{2} \int_{Q_{i}} \alpha_{i} \nabla u_{i} \cdot \nabla v \, dx \, dt = \int_{Q} f v \, dx \, dt$$

for all $v \in H^{1,0}_0(Q)
eq V_eta$

Remarks:

- ▶ Space-time (n+1 dimensional) formulation
- Final functions are discontinuous across Γ_* , test functions are not
- 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 .

$$\begin{split} & \mathcal{W}_n := \{ v : Q^n \to \mathbb{R} \mid v(x,t) = \phi_0(x) + t\phi_1(x), \quad \phi_0, \phi_1 \in V_n \} \\ & \mathcal{W} := \{ v : Q \to \mathbb{R} \mid v_{|Q^n} \in W_n \} \quad \text{(space-time FE)}. \end{split}$$



Approximating discontinuities

Space-time FE \Rightarrow Space-time XFEM

$$Q_{i}^{n} := \bigcup_{t \in I_{n}} \Omega_{i}(t), \quad R_{i}^{n} : \text{ restriction to } Q_{i}^{n}$$
$$W_{n}^{\Gamma} := R_{1}^{n} W_{n} \oplus R_{2}^{n} W_{n}, \quad W^{\Gamma_{*}} := \{ v : Q \to \mathbb{R} \mid v_{|Q^{n}} \in W_{n}^{\Gamma} \}$$
$$t_{n}$$



Conforming part (strong form + part. int. on diffusion)

Bilinear forms (within time slab Q^n) I

$$a^{n}(u,v) = \sum_{i=1}^{2} \int_{Q_{i}^{n}} \left(\frac{\partial u_{i}}{\partial t} + \mathbf{w} \cdot \nabla u_{i} \right) \beta_{i} v_{i} + \alpha_{i} \beta_{i} \nabla u_{i} \cdot \nabla v_{i} \, dx \, dt$$

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Discontinuous Galerkin Upwind w.r.t. time:

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

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Discontinuous Galerkin Upwind w.r.t. time:

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Henry interface condition

 $W_n^{\Gamma} \not\subset W_{\beta}$ (non-conformity) \Rightarrow enforce condition $[\![\beta u]\!]_{\Gamma^*} = 0$ only weakly (Nitsche)

Nitsche method for Henry condition:

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

0



Space-time approach

Bilinear forms (within time slab Q^n) II

Nitsche method for Henry condition:

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



Nitsche method for Henry condition:

_

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

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

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

$$\to \dots - \sum_{i=1}^{2} \int_{\Gamma_{*}^{n}} \nu \{\alpha \nabla u \cdot \mathbf{n}\}_{\Gamma_{*}^{n}} \beta_{i} v \, ds$$

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

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

Nitsche method for Henry condition:

พ a

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

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

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

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

$$\rightarrow - \int_{\Gamma_{n}^{n}} \nu \{\alpha \nabla v \cdot \mathbf{n}\}_{\Gamma_{n}^{n}} [\beta u]_{\Gamma_{n}^{n}} \, ds \quad \mathbf{B} + \lambda h_{n}^{-1} \int_{\Gamma_{n}^{n}} \nu [\beta u]_{\Gamma_{n}^{n}} \, ds, \quad \mathbf{C}$$
with $\{\cdot\}_{\Gamma_{n}^{n}}$ suitable volume weighted average. $\lambda > 0$: stabilization parameter and $\nu = 1/\sqrt{1 + (\mathbf{w} \cdot \mathbf{n})^{2}}$: $\int_{t^{n-1}}^{t^{n}} \int_{\Gamma_{n}} f \, ds \, dt = \int_{\Gamma_{n}^{n}} \nu f \, ds,$

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

Two-Phase Mass Transport Space-time approach

Nitsche-DG-XFEM variational problem



global bilinearforms

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

Discrete problem

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

$$B(U, V) = f(V) \quad \text{for all} \quad V \in W^{\Gamma_*},$$

$$B(U, V) := a(U, V) + d(U, V) + N_{\Gamma_*}(U, V)$$

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Still allows for time stepping, i.e. solving time slab by time slab!

Space-time approach

Error analysis (results)



Theorem

Error analysis for linear (space+time) FE

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

Theorem

Error analysis for linear (space+time) FE

Error analysis (results)

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

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









Two-Phase Mass Transport Space-

Space-time approach

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

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

Remark on 3+1 dimensions

Quadrature in (3+1)D

- Tringulation consists of prism-4 elements
- Decompose prism-4 into four pentatopes (simplex-4)
- Decompose cut-pentatopes into uncut pentatopes (approximation of Γ_{*})
- 4D quadrature on uncut pentatopes
- (!) For realistic problems quadrature limits convergence to $\mathcal{O}(\Delta t^2)$

Implementation and numerical results

- First implementation in 3+1 dimesions exists
- At least second order convergence is validated
- For simple examples even third order is observed

Conclusion



Interface capturing and consequences

- Level-set approach, Eulerian frame
- Non-matching interface needs special care for space discretization
- Moving discontinuities needs special care for time discretization

Discretization concepts

- 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]

Conclusion



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 [space-time integrals ⇒ Composite quadrature in (n+1) D]

Thank you for your attention!

Decomposition into simplices

The reference element can be decomposed into simplices

The reference prism-4 \hat{Q}



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} and it's decomposition



Decomposition into simplices

The reference element can be decomposed into simplices

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



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

Slicing the pentatope

(Non-degerenated) Case 1:



Slicing the pentatope

(Non-degerenated) Case 2:



Slicing the pentatope

(Non-degerenated) Case 2:



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

Slicing the pentatope

(Non-degerenated) Case 2:



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

Decomposition of the hypertriangle into 6 pentatopes

