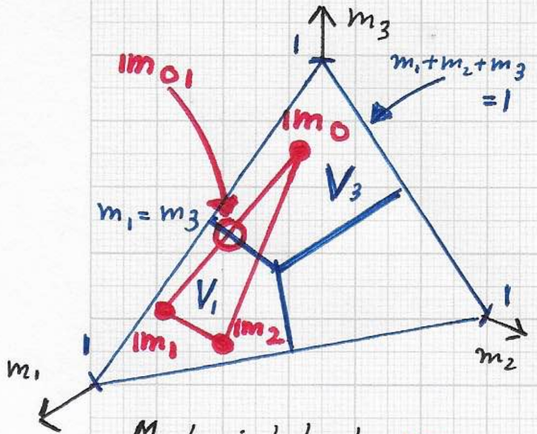
OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions: … Considering this specific example, the material interface found – i.e., points on it and their connecting line segment – must be mapped to "physical space," to the 2-simplex having $\mathbb{m}_0$, $\mathbb{m}_1$, and $\mathbb{m}_2$ as vertex-associated material fractions.



Material tuples $\mathbb{m}_0$ and $\mathbb{m}_1$ lie in tiles V_3 and V_1, respectively. The point on the interface between V_1 and V_3 is obtained via intersecting a parametric line through $\mathbb{m}_0$ and $\mathbb{m}_1$ with the implicit hyperplane bisector

$$m_1 + m_2 + m_3 = 1,$$

$$\text{where } m_1 = m_3.$$

The resulting point is called $\mathbb{m}_{01}$ in "material space."

• Note. The three bisecting line segments shown in the interior of the triangle are (clipped parts of) the intersections of the plane defined as

$$m_1 + m_2 + m_3 = 1$$

with the three planes defined as

$$m_1 = m_2,$$
$$m_1 = m_3 \quad \text{and}$$
$$m_2 = m_3,$$

respectively.

• Note. The tile boundaries (of the "material space" Voronoi complex) are hyperplanes / hyperplane intersections in the interior of the simplex. These hyperplanes are PERPENDICULAR bisectors of line segments $\overline{\mathbb{m}_j \mathbb{m}_k}$. The characteristic of being perpendicular is lost when mapping to "physical space."

The figure (left, top) illustrates the data involved in calculating a material interface point called $\mathbb{m}_{01}$. We compute this point by intersecting a parametrically defined line with an implicitly defined hyperplane. First, we compute the parameter value of t – when using t as parameter for the line through $\mathbb{m}_0$ and $\mathbb{m}_1$ – associated with $\mathbb{m}_{01}$. Second, we use this parameter value to interpolate simplex vertices $\mathbb{p}_0$ and $\mathbb{p}_1$.

…

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions: ... For the example shown on the previous page, we obtain the line equation

$$\mathbb{m}(t) = \mathbb{m}_0 + t\,(\mathbb{m}_1 - \mathbb{m}_0)$$

$$\Leftrightarrow (m_1(t), m_2(t), m_3(t)) = (m_1, m_2, m_3)$$

$$= (m_1^0, m_2^0, m_3^0) + t\,(m_1^1 - m_1^0, m_2^1 - m_2^0, m_3^1 - m_3^0)$$

(Both $\mathbb{m}_0$ and $\mathbb{m}_1$ lie in the plane $m_1 + m_2 + m_3 = 1$.)

The implicit plane equation to use for the intersection computation is

$$m_1 = m_3 .$$

When inserting $m_1(t)$ and $m_3(t)$ into this implicit equation one obtains

$$m_1^0 + t\,(m_1^1 - m_1^0) = m_3^0 + t\,(m_3^1 - m_3^0)$$

$$\Leftrightarrow \quad t = \frac{m_3^0 - m_1^0}{(m_1^1 - m_1^0) - (m_3^1 - m_3^0)} =: t_I .$$

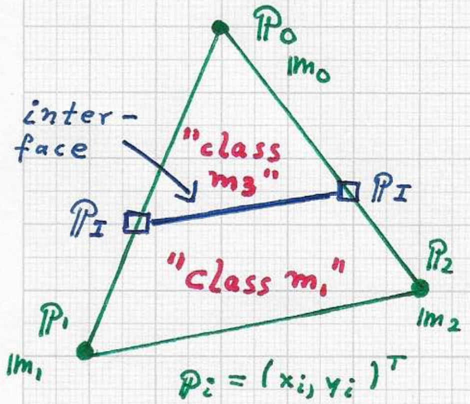
We call this parameter value, associated with the point $\mathbb{m}_{01}$ in material space, t_I. (The actual material fractions of $\mathbb{m}_{01}$ are m_1, $1-2m_1$ and m_1 – since $m_3 = m_1$ and $m_2 = 1 - m_1 - m_3 = 1 - 2m_1$.)

The material triples $\mathbb{m}_0$ and $\mathbb{m}_1$ are associated with "physical space" points $\mathbb{p}_0$ and $\mathbb{p}_1$. The material interface point can now be computed as

$$\mathbb{p}_I = \mathbb{p}_0 + t_I\,(\mathbb{p}_1 - \mathbb{p}_0),$$

see figure (left).

...



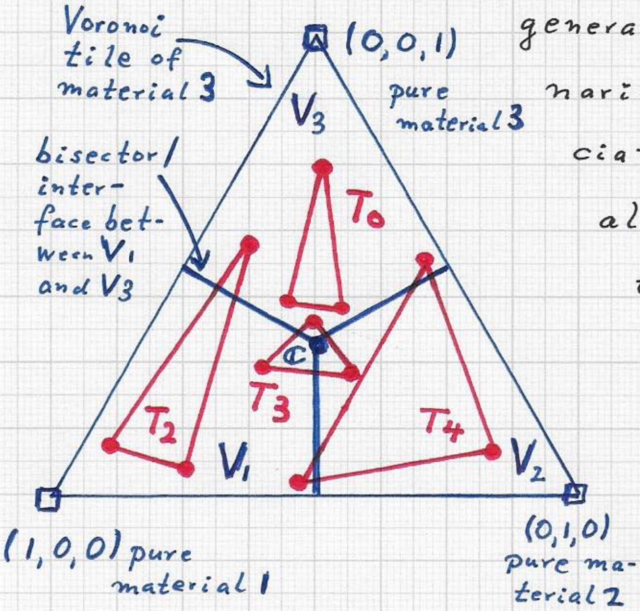
$\mathbb{p}_i = (x_i, y_i)^T$

$\mathbb{m}_i = (m_1^i, m_2^i, m_3^i)$

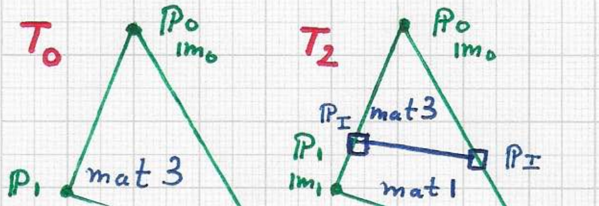
This "physical space" sketch relates to the figure on p. 15 (3/22/22). This 2-simplex has material triples $\mathbb{m}_i$ associated with its vertices. In this example, the 3 material triples lie in 2 different Voronoi tiles of the "pure" material triples (1,0,0), (0,1,0) and (0,0,1) in "material space." Here, $\mathbb{m}_0$ resides in the tile of the "pure" triple (0,0,1), while $\mathbb{m}_1$ and $\mathbb{m}_2$ reside in the tile of the "pure" triple (1,0,0). Thus, we first compute 2 interface points in "material space"; in a second step, we map these 2 points to the wanted material interface point in "physical space" – called $\mathbb{p}_I$ in the figure.

In the case of a 2-simplex, and ignoring possible singular and degenerate cases, the number of material interface points on the boundary of the 2-simplex can be 0, 2, 3 or 4.

■ OBJECT AND MATERIAL EIGENFUNCTIONS - Cont'd.



Possible configurations in "material space": material triples lying in various Voronoi tiles of three materials.



Mapping material interface points from "material space" back to "physical space" generates the points $\mathbb{P}_I$ shown for the four possible cases.

• Laplacian eigenfunctions: ... Ignoring all possible singular and degenerate cases, the 2-simplex scenario with material triples associated with the simplex vertices already generates several cases to be handled for material interface construction. The figure (left) sketches the combinatorially possible situations. In the shown "material space," a triangle defined by three material triples can belong to one of four types:

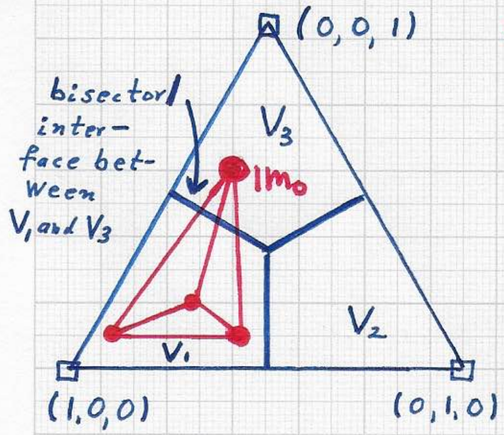
i) T_0 does not intersect a Voronoi tile boundary. T_0 is associated with one material class only.

ii) T_2 has three corner points in two Voronoi tiles. T_2 has 2 intersection points with one tile boundary; it is associated with 2 material classes.

iii) T_3 has three corner points in three Voronoi tiles. T_3 contains the Voronoi vertex $\mathbb{C}$. T_3 has 3 intersection points with 3 tile boundaries; it is ...

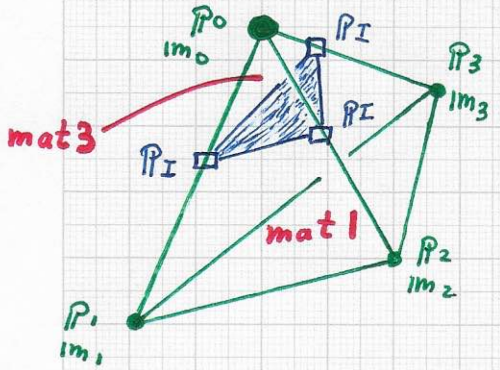
OBJECT AND MATERIAL EIGENFUNCTIONS - Cont'd.

• Laplacian eigenfunctions: ... associated with 3 material classes.



iv) T_4 has three corner points in three Voronoi tiles. T_4 DOES NOT contain the Voronoi vertex $\mathbb{C}$. T_4 has 4 intersection points with 2 tile boundaries (2 intersection points for each of the 2 tile boundaries); it is associated with 3 material classes.

"Flat 3-simplex" in "material space" resulting from the 4 vertex-associated material triples, $\mathbb{m} = (m_1, m_2, m_3)$. Three of the "flat 3-simplex" edges intersect the material bisector separating Voronoi tiles V_1 and V_3.



Mapping the three interface points to "physical space" produces points $\mathbb{P}_I$. By connecting these points on obtains the "postulated" interface triangle. This triangle separates the materia-1 from the material-3 region inside the 3-simplex.

The figures (previous page, top and bottom) sketch the four possible non-degenerate configurations in "material" and "physical space" that can occur for a 2-simplex with vertex-associated material fraction triples $\mathbb{m} = (m_1, m_2, m_3)$.

In the context of computational simulations of physical phenomena, 3-simplices are (generally) the simplices of highest dimension needed - especially for **VOLUME** fraction computations. Of course, the number of distinct materials considered is typically much larger than three. The figures shown on this page only serve the purpose of hinting at the combinatorial and geometrical complexity one must handle in the case of three materials and 3-simplex physical domains.

...

OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions: ... Since our driving problem is a multi-class data classification problem, we briefly sketch some of the concepts one must handle when defining and calculating (and representing) interfaces for multi-material data. In the general case of k materials/material classes, a material fraction tuple is

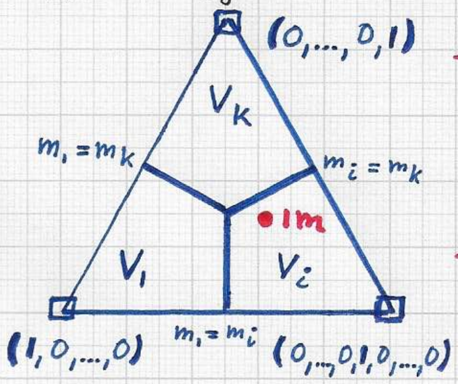
$$\mathbb{m} = (m_1, \ldots, m_k), \text{ where}$$
$$m_1 + \ldots + m_k = 1 \text{ and } m_i \geq 0.$$

In "material space" the k "pure" materials have k-tuples $(1,0,0,\ldots,0)$, $(0,1,0,\ldots,0)$, ... and $(0,0,0,\ldots,1)$. Again, one can associate a Voronoi tile with each of these k "pure" materials. The number of Voronoi tiles is k, and all k tiles have the same geometry. Tile boundaries are hyper-planes (i.e., parts of hyperplanes) that are perpendicular bisectors and define material interfaces. The set of all hyper-planes is defined by

$$m_i = m_j, \quad 1 \leq i < j \leq k.$$

Thus, the number of hyper-planes is $\binom{k}{2}$. The value of $\binom{k}{2}$ is $\frac{1}{2}(k^2 - k)$, i.e., the number of of hyper-planes grows quadratically with the number of materials.

...



Simplied illustration of the general k-material case and the Voronoi-based tessellation of "material space" with geometrically identical Voronoi tiles $V_1, \ldots, V_k$.

In the interior of the allowable "material space" domain Voronoi tile V_i is bounded by (parts of) the (k-1) hyper-planes defined by $m_i = m_1, \ldots, m_i = m_{i-1}, m_i = m_{i+1}, \ldots, m_i = m_k$.

In the context having to CLASSIFY A MATERIAL TUPLE $\mathbb{m}$, we must consider the following properties:

1) Tuple $\mathbb{m}$ is in V_i when the unique material tuple $(0,\ldots,0,1,0,\ldots,0)$ is $\mathbb{m}$'s closest "pure" material tuple.

2) Tuple $\mathbb{m}$ lies on a (multiple) bisector(s) when two (or more) of its m-values are equal.

!