

Implementation of HDG in three dimensions

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Notation of this documentation follows strictly that of the paper

Matlab tools for HDG in three dimensions

1 Pseudo-Matlab notation

Assume that \mathbf{u} is a column vector with N components and A is an $M \times N$ matrix. We then consider the $M \times N$ matrix $\mathbf{u}^\top \odot A := A \text{diag}(\mathbf{u})$ with elements

$$(\mathbf{u}^\top \odot A)_{ij} = u_j A_{ij}.$$

Similarly, if \mathbf{v} is a column vector with M components, we consider the matrix $\mathbf{v} \odot A := \text{diag}(\mathbf{v})A$, i.e.,

$$(\mathbf{v} \odot A)_{ij} = v_i A_{ij}.$$

Assuming correct sizes for the matrices and vectors (vectors will be assumed to be column vectors throughout), both operations can be easily accomplished in Matlab

```
bsxfun(@times,u',A)    % row times matrix
bsxfun(@times,v,A)     % column times matrix
```

We will use Kronecker products in a very particular form. Assume that \mathbf{c} is a column vector with N components and that A is a $m \times n$ matrix. Then

$$\mathbf{c}^\top \otimes A = [c_1 A \mid c_2 A \mid \cdots \mid c_N A]$$

is a $m \times (nN)$ matrix, organized in N blocks of size $m \times n$. It will be the case that we will want the result stored as a 3-dimensional $m \times n \times N$. This is easily programmed as follows

```
cA=kron(c',A);
cA=reshape(cA,[m,n,N]);
```

For convenience, we will also write

$$\mathbf{a}_i^\top := \text{row}(A, i)$$

to select the i -th row of a matrix A . Finally, in the last part of the code we will use the symbol \bullet to represent the element by element multiplication of arrays (Matlab's \cdot operator).

2 Geometric elements

2.1 Reference elements

We first consider the reference tetrahedron \widehat{K} , with vertices

$$\widehat{\mathbf{v}}_1 := (0, 0, 0) \quad \widehat{\mathbf{v}}_2 := (1, 0, 0), \quad \widehat{\mathbf{v}}_3 := (0, 1, 0), \quad \widehat{\mathbf{v}}_4 := (0, 0, 1).$$

Note that $|\widehat{K}| := \text{vol } \widehat{K} = 1/6$. We also consider the two dimensional reference element $\widehat{K}_2 := \{(s, t) : s, t \geq 0, s + t \leq 1\}$ with vertices

$$\widehat{\mathbf{w}}_1 := (0, 0), \quad \widehat{\mathbf{w}}_2 := (1, 0), \quad \widehat{\mathbf{w}}_3 := (0, 1).$$

2.2 Tetrahedra

Given a tetrahedron with vertices $(\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, \mathbf{v}_4)$ (the order is relevant), we consider the affine mapping $F_K : \widehat{K} \rightarrow K$

$$F_K(\widehat{\mathbf{x}}) = B_K \widehat{\mathbf{x}} + \mathbf{v}_1, \quad B_K = \begin{bmatrix} x_2 - x_1 & x_3 - x_1 & x_4 - x_1 \\ y_2 - y_1 & y_3 - y_1 & y_4 - y_1 \\ z_2 - z_1 & z_3 - z_1 & z_4 - z_1 \end{bmatrix}$$

so that $F_K(\widehat{\mathbf{v}}_i) = \mathbf{v}_i$ for $i \in \{1, 2, 3, 4\}$. All elements of the triangulation will be given with positive orientation, that is,

$$\det B_K = 6|K| = \left((\mathbf{v}_2 - \mathbf{v}_1) \times (\mathbf{v}_3 - \mathbf{v}_1) \right) \cdot (\mathbf{v}_4 - \mathbf{v}_1) > 0.$$

2.3 Parametrization of triangles

A triangle e in \mathbb{R}^3 with vertices $(\mathbf{w}_1, \mathbf{w}_2, \mathbf{w}_3)$ (the order is relevant), will be parametrized via $\phi_e : \widehat{K}_2 \rightarrow e$, given by

$$\phi_e(s, t) := s(\mathbf{w}_2 - \mathbf{w}_1) + t(\mathbf{w}_3 - \mathbf{w}_1) + \mathbf{w}_1, \quad |\partial_s \phi_e \times \partial_t \phi_e| = 2|e|,$$

so that $\phi_e(\widehat{\mathbf{w}}_i) = \mathbf{w}_i$, for $i \in \{1, 2, 3\}$. The local orientation of the vertices of e gives an orientation to the normal vector: we will define the normal vector so that its norm is proportional to the area of e , that is

$$\mathbf{n}_e := \frac{1}{2} \left((\mathbf{w}_2 - \mathbf{w}_1) \times (\mathbf{w}_3 - \mathbf{w}_1) \right).$$

2.4 Parametrization of the faces of a tetrahedron

Given a tetrahedron K with vertices $(\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, \mathbf{v}_4)$ we will consider its four faces given in the following order (and with the inherited orientations):

$$\begin{array}{llll} e_1^K & \longleftrightarrow & (\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3) & \begin{bmatrix} 1 & 2 & 3 \\ 1 & 2 & 4 \\ 1 & 3 & 4 \\ 4 & 2 & 3 \end{bmatrix} \\ e_2^K & \longleftrightarrow & (\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_4) & \\ e_3^K & \longleftrightarrow & (\mathbf{v}_1, \mathbf{v}_3, \mathbf{v}_4) & \\ e_4^K & \longleftrightarrow & (\mathbf{v}_4, \mathbf{v}_2, \mathbf{v}_3). & \end{array}$$

(Note that with this orientation of the faces, the normals of the second and fourth faces point outwards, while those of the first and third faces point inwards. This numbering is done for the sake of parametrization.)

The parametrizations of the faces $e_\ell^K \in \mathcal{E}(K)$

$$\phi_\ell^K : \widehat{K}_2 \rightarrow e_\ell^K \quad \ell \in \{1, 2, 3, 4\},$$

given by the formulas

$$\phi_1^K(s, t) := (s, t, 0)$$

$$\phi_2^K(s, t) := (s, 0, t)$$

$$\phi_3^K(s, t) := (0, s, t)$$

$$\phi_4^K(s, t) := (s, t, 1 - s - t)$$

will be used for integrals on ∂K .

2.5 The permutation index

Consider the affine invertible maps $F_\mu : \widehat{K}_2 \rightarrow \widehat{K}_2$ given by the formulas

$$\begin{array}{ll} F_1(s, t) := (s, t) & \left[\begin{array}{ccc} \mathbf{1} & \mathbf{2} & \mathbf{3} \\ 1 & 3 & 2 \\ 3 & 1 & 2 \\ 3 & \mathbf{2} & 1 \\ 2 & 3 & 1 \\ 2 & 1 & \mathbf{3} \end{array} \right] \\ F_2(s, t) := (t, s) & \\ F_3(s, t) := (t, 1 - s - t) & \\ F_4(s, t) := (s, 1 - s - t) & \\ F_5(s, t) := (1 - s - t, s) & \\ F_6(s, t) := (1 - s - t, t) & \end{array} .$$

The table on the right shows the indices of images of the vertices ($\widehat{\mathbf{w}}_1, \widehat{\mathbf{w}}_2, \widehat{\mathbf{w}}_3$), with boldface font for those that stay fixed. We note that F_2, F_4 and F_6 change orientation.

Given a tetrahedron K , assume that the face $e = e_\ell^K$. We thus have six possible cases of how the parametrizations ϕ_ℓ^K and ϕ_e match. We will encode this information in a matrix so that

$$\mu = \text{perm}(K, \ell) \quad \text{and} \quad e = e_\ell^K \quad \text{imply} \quad \phi_e \circ F_\mu = \phi_\ell^K .$$

2.6 A tetrahedrization in basic and expanded forms

We are given a polyhedral domain Ω , with faces grouped in two subsets Γ_D and Γ_N (for Dirichlet and Neumann boundary conditions), and a tetrahedrization of Ω . The basic tetrahedrization is given through four fields:

- **T.coordinates** is an $N_{\text{ver}} \times 3$ matrix with the coordinates of the vertices of the triangulation,
- **T.elements** is an $N_{\text{elt}} \times 4$ matrix: the K -th row of the matrix contains the indices of the vertices of K ; *positive orientation is assumed*,
- **T.dirichlet** is a $N_{\text{dir}} \times 3$ matrix, with the vertex numbers for the Dirichlet faces,
- **T.neumann** is a $N_{\text{neu}} \times 3$ matrix, with the vertex numbers for the Neumann faces.

For the boundary faces, it is assumed that *either all of them are given with positive orientation* (normals pointing outwards) or *all of them are given with negative orientation*. This is an example of a basic tetrahedral data structure, for a partition with 48 vertices, 108 tetrahedral elements, 36 Dirichlet faces and 48 Neumann faces.

```
T =
  coordinates: [48x3 double]
  elements: [108x4 double]
  dirichlet: [36x3 double]
  neumann: [48x3 double]
```

In **expanded form**, the tetrahedral data structure contains many more useful fields.

- In this form, the faces listed in the fields **T.dirichlet** and **T.neumann** are positively oriented.
- **T.faces** is a $N_{\text{fc}} \times 4$ matrix with a list of faces: the first three columns contain the global vertex numbers for the faces (its order will give the intrinsic parametrization of the face); Dirichlet and Neumann faces are numbered exactly as in **T.dirichlet** and **T.neumann**, the fourth column contains an index:

- 0 for interior faces
- 1 for Dirichlet faces
- 2 for Neumann faces
- **T.dirfaces** and **T.neufaces** are row vectors with the list of Dirichlet and Neumann faces (that is, they point out what rows of **T.faces** contain a 1 (resp a 2) in the last column)
- **T.facebyele** is an $N_{\text{elt}} \times 4$ matrix: its K -th row contains the numbers of faces that make up ∂K ; they are given in the order shown in Section 2.4, that is, locally

$$\begin{bmatrix} 1 & 2 & 3 \\ 1 & 2 & 4 \\ 1 & 3 & 4 \\ 4 & 2 & 3 \end{bmatrix}$$

This is the matrix we have described as e_ℓ^K .

- **T.perm** is an $N_{\text{elt}} \times 4$ matrix containing numbers from 1 to 6; the K -th row indicates what permutations are needed for each of the faces to get to the proper numbering of the face (see Section 2.5), i.e., this is just the matrix $\text{perm}(K, \ell)$
- **T.volume** is a $N_{\text{elt}} \times 1$ column vector with the volumes of the elements
- **T.area** is a $N_{\text{fc}} \times 1$ column vector with the areas of the faces
- **T.normals** is a $N_{\text{elt}} \times 12$ matrix with the *non-normalized* normal vectors for the faces of the ech; its K -th row contains four row vectors of three components each

$$[\mathbf{n}_1^\top \mid \mathbf{n}_2^\top \mid \mathbf{n}_3^\top \mid \mathbf{n}_4^\top]$$

so that \mathbf{n}_ℓ is the normal vector to the face e_ℓ^K , *pointing outwards* and such that $|\mathbf{n}_\ell| = |e_\ell^K|$.

```
T =
coordinates: [48x3 double]
elements: [108x4 double]
dirichlet: [36x3 double]
neumann: [48x3 double]
faces: [258x4 double]
dirfaces: [1x36 double]
neufaces: [1x48 double]
facebyele: [108x4 double]
orientation: [108x4 double]
perm: [108x4 double]
volume: [108x1 double]
area: [258x1 double]
normals: [108x12 double]
```

In what follows we will frequently identify

$$\mathcal{T}_h \equiv \{1, \dots, N_{\text{elt}}\} \quad \mathcal{E}_h \equiv \{1, \dots, N_{\text{fc}}\}.$$

3 Quadrature

3.1 Volume integrals

Quadrature rules will be given in the reference element \widehat{K} . They will be composed of quadrature points, given by their *barycentric coordinates*, and weights. Geometrically, we can think of points

$$\widehat{\mathbf{p}}_q := (\widehat{x}_q, \widehat{y}_q, \widehat{z}_q), \quad q = 1, \dots, N_{\text{qd}}$$

and weights $\widehat{\omega}_q$, with the normalization

$$\sum_{q=1}^{N_{\text{qd}}} \widehat{\omega}_q = 1, \quad \text{so that} \quad \int_{\widehat{K}} \widehat{\phi} \approx \frac{1}{6} \sum_q \widehat{\omega}_q \widehat{\phi}(\widehat{\mathbf{p}}_q).$$

For a general tetrahedron, we will approximate

$$\int_K \phi = \det \mathbf{B}_K \int_{\widehat{K}} \phi \circ \mathbf{F}_K \approx |K| \sum_q \widehat{\omega}_q \phi(\mathbf{p}_q^K) \quad \text{with} \quad \mathbf{p}_q^K = \mathbf{F}_K(\widehat{\mathbf{p}}_q).$$

For convenience, a quadrature formula will be stored in an $N_{\text{qd}} \times 5$ matrix. The q -th row contains the barycentric coordinates of $\widehat{\mathbf{p}}_q$ and then the weight $\widehat{\omega}_q$, that is, we store

$$(1 - \widehat{x}_q - \widehat{y}_q - \widehat{z}_q, \widehat{x}_q, \widehat{y}_q, \widehat{z}_q, \widehat{\omega}_q)$$

as rows. We will also consider the $N_{\text{qd}} \times 4$ matrix Λ with the barycentric coordinates of the quadrature points.

3.2 Integrals on faces

Two dimensional quadrature rules will be given in the reference element \widehat{K}_2 , using points and weights so that

$$\sum_{r=1}^{N_{\text{qd}2}} \varpi_r = 1 \quad \text{and thus} \quad \int_{\widehat{K}_2} \widehat{\phi} \approx \frac{1}{2} \sum_r \varpi_r \widehat{\phi}(\widehat{\mathbf{q}}_r), \quad \widehat{\mathbf{q}}_r = (\widehat{s}_r, \widehat{t}_r).$$

To compute an integral on $e \in \mathcal{E}_h$, we simply parametrize from \widehat{K}_2 and proceed accordingly:

$$\int_e \phi = 2|e| \int_{\widehat{K}_2} \phi \circ \phi_e \approx |e| \sum_r \varpi_r \phi(\mathbf{q}_r^e) \quad \text{with} \quad \mathbf{q}_r^e := \phi_e(\widehat{\mathbf{q}}_r).$$

A face quadrature formula will be stored in an $N_{\text{qd}2} \times 4$ matrix, with the barycentric coordinates of the quadrature points in the first columns and the weights in the last one. The r -th row of this matrix is therefore

$$(1 - \widehat{s}_r - \widehat{t}_r, \widehat{s}_r, \widehat{t}_r, \varpi_r).$$

The $N_{\text{qd}2} \times 3$ with the barycentric coordinates of the quadrature points will be denoted Ξ .

3.3 Integrals on boundaries of tetrahedra

In many cases we will be integrating on a face that is given with geometric information of an adjacent tetrahedron. The quadrature points $\widehat{\mathbf{q}}_r$ lead to four groups of quadrature points on the faces of \widehat{K} (see Section 2.4):

$$\begin{aligned} \widehat{\mathbf{q}}_r^1 &:= (\widehat{s}_r, \widehat{t}_r, 0) \\ \widehat{\mathbf{q}}_r^2 &:= (\widehat{s}_r, 0, \widehat{t}_r) \\ \widehat{\mathbf{q}}_r^3 &:= (0, \widehat{s}_r, \widehat{t}_r) \\ \widehat{\mathbf{q}}_r^4 &:= (\widehat{s}_r, \widehat{t}_r, 1 - \widehat{s}_r - \widehat{t}_r) \end{aligned}$$

For a given $\psi : K \rightarrow \mathbb{R}$, we can approximate

$$\int_{e_\ell^K} \psi \approx |e_\ell^K| \sum_r \varpi_r \psi(\mathbf{q}_{r,\ell}^K) \quad \text{with} \quad \mathbf{q}_{r,\ell}^K = F_K(\hat{\mathbf{q}}_r^\ell) = \phi_{e_\ell^K}(F_{\text{perm}(K,\ell)}(\hat{\mathbf{q}}_r))$$

and thus

$$\int_{\partial K} \psi \approx \sum_{\ell=1}^4 |e_\ell^K| \sum_r \varpi_r \psi(\mathbf{q}_{r,\ell}^K).$$

4 Dubiner polynomial bases

4.1 The Dubiner basis in two variables

Let

$$d_2 = d_2(k) = \binom{k+2}{2} = \dim \mathcal{P}_k(\hat{K}_2).$$

The Dubiner basis in two variables is a basis of the space of bivariate polynomials such that

$$\int_{\hat{K}_2} \check{D}_i \check{D}_j = 0 \quad i \neq j, \quad \check{K}_2 = \{2\hat{\mathbf{x}} - (1,1)^\top : \hat{\mathbf{x}} \in \hat{K}_2\}.$$

It is ordered in such a way that

$$\mathcal{P}_k(\check{K}_2) = \text{span}\{\check{D}_j : j \leq d_2(k)\} \quad \forall k \geq 0.$$

The Dubiner basis is evaluated using Jacobi polynomials (here we use a small variation of code by John Buckhart for the evaluation of the Jacobi polynomials). Details on how this is coded can be found in the documentation of the 2-dimensional HDG code. Given N_{points} points $\mathbf{q}_r = (s_r, t_r)$, the function `dubiner2d` returns the matrices

$$\check{D}_j(\mathbf{q}_r), \quad \partial_s \check{D}_j(\mathbf{q}_r), \quad \partial_t \check{D}_j(\mathbf{q}_r).$$

Output is given as three $N_{\text{points}} \times d_2$ matrices.

```
function [db,dbx,dby]=dubiner2d(x,y,k)
% function [db,dbx,dby]=dubiner2d(x,y,k)
% input:
%     x,y: the coordinates at which we evaluate the Dubiner basis
%     k: the degree of the polynomial. Must be a column vector.
% output:
%     db: the value of dubiner basis at given coordinates, Nnodes x Nbasis
%     dbx: the derivative to x of the Dubiner basis, Nnodes x Nbasis
%     dby: the derivative to y of the Dubiner basis, Nnodes x Nbasis
%
% Last modified: June 5 2012

Nnodes=size(x,1);
Nbasis=nchoosek(k+2,2);
db=zeros(Nnodes,Nbasis);
dbx=zeros(Nnodes,Nbasis);
dby=zeros(Nnodes,Nbasis);
etal(y~=1)=2*(1+x(y~=1))./(1-y(y~=1))-1;
etal(y==1)=-1; etal=etal';
eta2=y;
% locate the index with p,q
a=zeros(k+1,k+1);
index=1;
for l=2:k+2
    for i=l-1:-1:1
```

```

        a(i,l-i)=index;
        index=index+1;
    end
end
loc=@(p,q) a(p+1,q+1);
%
% Dubiner Basis
JP=JacobiP(k,0,0,eta1);
for p=0:k
    A=JP(:,p+1).*((1-eta2)/2).^p;
    JPQ=JacobiP(k-p,2*p+1,0,eta2);
    for q=0:k-p
        db(:,loc(p,q))=A.*JPQ(:,q+1);
    end
end
%
% Derivative of Dubiner Basis
dbx(:,loc(0,0))=0.*x;          % DB_x^{0,0}
dby(:,loc(0,0))=0.*y;          % DB_y^{0,0}
if k>0
    dbx(:,loc(1,0))=1+0.*x;      % DB_x^{1,0}
    dby(:,loc(1,0))=1/2+0.*y;    % DB_y^{1,0}
end
for p=1:k-1
    dbx(:,loc(p+1,0))=(2*p+1)/(p+1)*(1+2.*x+y)/2.*dbx(:,loc(p,0))....
        -p/(p+1)*(1-y).^2/4.*dbx(:,loc(p-1,0))....
        +(2*p+1)/(p+1)*db(:,loc(p,0));
    dby(:,loc(p+1,0))=1/2*(2*p+1)/(p+1)*db(:,loc(p,0))....
        +(2*p+1)/(p+1)*(1+2*x+y)/2.*dby(:,loc(p,0))....
        -p/(p+1)*(1/2*(y-1).*db(:,loc(p-1,0))+(1-y).^2/4.*dby(:,loc(p-1,0)));
end
for p=0:k-1
    dbx(:,loc(p,1))=dbx(:,loc(p,0)).*(1+2*p+(3+2*p)*y)/2;
    dby(:,loc(p,1))=dby(:,loc(p,0)).*(1+2*p+(3+2*p)*y)/2+(3+2*p)/2*db(:,loc(p,0));
end
for p=0:k-1
    for q=1:k-p-1
        a=(2*q+2*p+2)*(2*q+2*p+3)/2/(q+1)/(q+2*p+2);
        b=(2*q+2*p+2)*(2*p+1)^2/2/(q+1)/(q+2*p+2)/(2*q+2*p+1);
        c=(2*q+2*p+3)*(q+2*p+1)*q/(q+1)/(q+2*p+2)/(2*q+2*p+1);
        dbx(:,loc(p,q+1))=(a*y+b).*dbx(:,loc(p,q))-c*dbx(:,loc(p,q-1));
        dby(:,loc(p,q+1))=(a*y+b).*dby(:,loc(p,q))-c*dby(:,loc(p,q-1))+a*db(:,loc(p,q));
    end
end
return

function v = JacobiP(n,alpha,beta,x)

% Subfunction with evaluation of Jacobi polynomials
% taken from code by John Burkardt,
% distributed under the GNU LGPL license

v=zeros(size(x,1),n+1);
v(:,1) = 1.0;
if ( n == 0 )
    return
end

v(:,2) = ( 1.0 + 0.5 * ( alpha + beta ) ) * x(:) + 0.5 * ( alpha - beta );

for i = 2 : n
    c1 = 2 * i * ( i + alpha + beta ) * ( 2 * i - 2 + alpha + beta );
    c2 = ( 2 * i - 1 + alpha + beta ) * ( 2 * i + alpha + beta ) ...
        * ( 2 * i - 2 + alpha + beta );

```

```

c3 = ( 2 * i - 1 + alpha + beta ) * ( alpha + beta ) * ( alpha - beta );
c4 = - 2 * ( i - 1 + alpha ) * ( i - 1 + beta ) * ( 2 * i + alpha + beta );
v(:,i+1) = ( ( c3 + c2 * x(:) ) .* v(:,i) + c4 * v(:,i-1) ) / c1;
end

return

```

4.2 The Dubiner basis in three variables

We now denote

$$d_3 := d_3(k) = \binom{k+3}{3} = \dim \mathcal{P}_k(\widehat{K}).$$

A basis $\{\check{P}_j\}$ of the space of 3-variate polynomials is given with the orthogonality property

$$\int_{\check{K}} \check{P}_i \check{P}_j = 0 \quad i \neq j, \quad \check{K} = \{2\widehat{\mathbf{x}} - (1,1,1)^\top : \widehat{\mathbf{x}} \in \widehat{K}\}.$$

We also assume that

$$\mathcal{P}_k(\check{K}) = \text{span}\{P_j : j \leq d_3(k)\} \quad \forall k \geq 0.$$

Output is given in a similar way to the `dubiner2d` code: given points \mathbf{p}_q , we evaluate

$$\check{P}_j(\mathbf{p}_q), \quad \partial_x \check{P}_j(\mathbf{p}_q), \quad \partial_y \check{P}_j(\mathbf{p}_q), \quad \partial_z \check{P}_j(\mathbf{p}_q)$$

and output as four $N_{\text{points}} \times d_3$ matrices.

```

function [db,dbx,dbz]=dubiner3d(x,y,z,k)
% function [db,dbx,dbz]=dubiner3d(x,y,z,k)
% input:
%   x,y,z: the coordinates at which we evaluate the Dubiner basis
%   k: the degree of the polynomial. Must be a column vector.
% output:
%   db: the value of dubiner basis at given coordinates, Nnodes x Nbasis
%   dbx: the derivative to x of the Dubiner basis, Nnodes x Nbasis
%   dby: the derivative to y of the Dubiner basis, Nnodes x Nbasis
%   dbz: the derivative to y of the Dubiner basis, Nnodes x Nbasis
% Last modified: May 16 2012

Nnodes=size(x,1);
Nbasis=nchoosek(k+3,3);
db=zeros(Nnodes,Nbasis);
dbx=zeros(Nnodes,Nbasis);
dby=zeros(Nnodes,Nbasis);
dbz=zeros(Nnodes,Nbasis);
a=@(al,be,n) ( (2*n+1+al+be)*(2*n+2+al+be) ) / ( 2*(n+1)*(n+1+al+be) );
b=@(al,be,n) ( (al^2-be^2)*(2*n+1+al+be) ) / ( 2*(n+1)*(2*n+al+be)*...
                                                (n+1+al+be) );
c=@(al,be,n) ( (n+al)*(n+be)*(2*n+2+al+be) ) / ( (n+1)*(n+1+al+be)*...
                                                (2*n+al+be) );

% Locate the basis with index p,q,r
index=zeros(k+1,k+1,k+1);
count=1;
%
for j=0:k
    for i1=j:-1:0
        for i2=j-i1:-1:0
            index(i1+1,i2+1,j-i1-i2+1)=count;
            count=count+1;
        end
    end
end
end

```

```

end
loc=@(i1,i2,i3) index(i1+1,i2+1,i3+1);

F1= (2+2*x+y+z)/2;   F1x= 1+0*x;   Fly= 1/2+0*x;   F1z= 1/2+0*x;
F2= ((y+z)/2).^2;    F2x= 0.*x;    F2y= 1/2*(y+z); F2z= 1/2*(y+z);
F3= (2+3*y+z)/2;     F3x= 0+0.*x;   F3y= 3/2+0.*x; F3z= 1/2+0.*x;
F4= (1+2*y+z)/2;     F4x= 0+0.*x;   F4y= 1+0.*x;   F4z= 1/2+0.*x;
F5= (1-z)/2;         F5x= 0+0.*x;   F5y= 0+0.*x;   F5z= -1/2+0.*x;

db(:,loc(0,0,0))=1;
dbx(:,loc(0,0,0))=0*x;   dbx(:,loc(0,0,0))=0*y;   dbz(:,loc(0,0,0))=0*z;
if k>0
    db(:,loc(1,0,0))=F1;
    dbx(:,loc(1,0,0))=F1x; dbx(:,loc(1,0,0))=F1y; dbz(:,loc(1,0,0))=F1z;
end
for p=1:k-1
    db(:,loc(p+1,0,0))=(2*p+1)/(p+1)*F1.*db(:,loc(p,0,0))....
        -(p/(p+1))*F2.*db(:,loc(p-1,0,0));
    dbx(:,loc(p+1,0,0))=(2*p+1)/(p+1)*( F1x.*db(:,loc(p,0,0)) + ...
        F1.*dbx(:,loc(p,0,0)) ) - (p/(p+1))*( F2x.*db(:,loc(p-1,0,0))+ ...
        F2.*dbx(:,loc(p-1,0,0)) );
    dbx(:,loc(p+1,0,0))=(2*p+1)/(p+1)*( Fly.*db(:,loc(p,0,0)) + ...
        F1.*dbx(:,loc(p,0,0)) ) - (p/(p+1))*( F2y.*db(:,loc(p-1,0,0))+ ...
        F2.*dbx(:,loc(p-1,0,0)) );
    dbz(:,loc(p+1,0,0))=(2*p+1)/(p+1)*( F1z.*db(:,loc(p,0,0)) + ...
        F1.*dbz(:,loc(p,0,0)) ) - (p/(p+1))*( F2z.*db(:,loc(p-1,0,0))+ ...
        F2.*dbz(:,loc(p-1,0,0)) );
end

for p=0:k-1
    db(:,loc(p,1,0))=(p*(1+y)+F3).*db(:,loc(p,0,0));
    dbx(:,loc(p,1,0)) = F3x.*db(:,loc(p,0,0)) +...
        dbx(:,loc(p,0,0)).*(p*(1+y)+F3);
    dbx(:,loc(p,1,0)) = (p+F3y).*db(:,loc(p,0,0)) +...
        dbx(:,loc(p,0,0)).*(p*(1+y)+F3);
    dbz(:,loc(p,1,0)) = F3z.*db(:,loc(p,0,0)) +...
        dbz(:,loc(p,0,0)).*(p*(1+y)+F3);
end

for p=0:k-2
    for q=1:k-p-1
        db(:,loc(p,q+1,0))=(a(2*p+1,0,q)*F4+b(2*p+1,0,q)*F5).*db(:,loc(p,q,0))....
            -c(2*p+1,0,q)*F5.^2.*db(:,loc(p,q-1,0));
        dbx(:,loc(p,q+1,0))=(a(2*p+1,0,q)*F4x+b(2*p+1,0,q)*F5x).*db(:,loc(p,q,0))....
            +(a(2*p+1,0,q)*F4+b(2*p+1,0,q)*F5).*dbx(:,loc(p,q,0))....
            -2*c(2*p+1,0,q)*F5.*F5x.*db(:,loc(p,q-1,0))....
            -c(2*p+1,0,q)*F5.^2.*dbx(:,loc(p,q-1,0));
        dbx(:,loc(p,q+1,0))=(a(2*p+1,0,q)*F4y+b(2*p+1,0,q)*F5y).*db(:,loc(p,q,0))....
            +(a(2*p+1,0,q)*F4+b(2*p+1,0,q)*F5).*dbx(:,loc(p,q,0))....
            -2*c(2*p+1,0,q)*F5.*F5y.*db(:,loc(p,q-1,0))....
            -c(2*p+1,0,q)*F5.^2.*dbx(:,loc(p,q-1,0));
        dbz(:,loc(p,q+1,0))=(a(2*p+1,0,q)*F4z+b(2*p+1,0,q)*F5z).*db(:,loc(p,q,0))....
            +(a(2*p+1,0,q)*F4+b(2*p+1,0,q)*F5).*dbz(:,loc(p,q,0))....
            -2*c(2*p+1,0,q)*F5.*F5z.*db(:,loc(p,q-1,0))....
            -c(2*p+1,0,q)*F5.^2.*dbz(:,loc(p,q-1,0));

        end
    end

for p=0:k-1
    for q=0:k-p-1
        db(:,loc(p,q,1)) =(1+p+q+(2+q+p)*z).*db(:,loc(p,q,0));
        dbx(:,loc(p,q,1)) =(1+p+q+(2+q+p)*z).*dbx(:,loc(p,q,0));
        dbx(:,loc(p,q,1)) =(1+p+q+(2+q+p)*z).*dbx(:,loc(p,q,0));
        dbz(:,loc(p,q,1)) =(1+p+q+(2+q+p)*z).*dbz(:,loc(p,q,0))....

```

```

        + (2+p+q)*db(:,loc(p,q,0));
    end
end
for p=0:k-2
    for q=0:k-p-2
        for r=1:k-p-q-1
            db(:,loc(p,q,r+1))=(a(2*p+2*q+2,0,r)*z+b(2*p+2*q+2,0,r)).*...
                db(:,loc(p,q,r))-c(2*p+2*q+2,0,r)*db(:,loc(p,q,r-1));
            dbx(:,loc(p,q,r+1))=(a(2*p+2*q+2,0,r)*z+b(2*p+2*q+2,0,r)).*...
                dbx(:,loc(p,q,r))-c(2*p+2*q+2,0,r)*dbx(:,loc(p,q,r-1));
            dby(:,loc(p,q,r+1))=(a(2*p+2*q+2,0,r)*z+b(2*p+2*q+2,0,r)).*...
                dby(:,loc(p,q,r))-c(2*p+2*q+2,0,r)*dby(:,loc(p,q,r-1));
            dbz(:,loc(p,q,r+1))=(a(2*p+2*q+2,0,r)*z+b(2*p+2*q+2,0,r)).*...
                dbz(:,loc(p,q,r))-c(2*p+2*q+2,0,r)*dbz(:,loc(p,q,r-1)).*...
                + a(2*p+2*q+2,0,r)*db(:,loc(p,q,r));
        end
    end
end
return

```

5 Volume matrices and integrals

5.1 Representation of a piecewise polynomial function

Let k be a fixed polynomial degree and consider

$$\hat{P}_j := \check{P}_j(2 \cdot -(1,1,1)^\top), \quad \mathcal{P}_k(\hat{K}) = \text{span}\{\hat{P}_j : 1 \leq j \leq d_3\}.$$

This basis is hierarchical. We then consider the following basis of $\mathcal{P}_k(K)$

$$P_i^K := \hat{P}_i \circ F_K^{-1}, \quad i = 1, \dots, d_3.$$

A function in the space

$$W_h := \prod_{K \in \mathcal{T}_h} \mathcal{P}_k(K) = \{u_h : \Omega \rightarrow \mathbb{R} : u_h|_K \in \mathcal{P}_k(K) \quad \forall K \in \mathcal{T}_h\}$$

will be represented in two possible forms: as a $d_3 \times N_{\text{elt}}$ matrix, whose K -th column contains the coefficients of $u_h|_K$ in the basis $\{P_i^K\}$, or as a $d_3 N_{\text{elt}}$ column vector, with d_3 -sized blocks containing the same values. *The matrix storage form will be preferred.* The **reshape** command moves from one to the other easily.

Warning. At every evaluation of the basis functions or their derivatives, we need to apply the following rule

$$\hat{P}_i(\mathbf{x}) = \check{P}_i(2\mathbf{x} - \mathbf{1}), \quad \partial_\star \hat{P}_i(\mathbf{x}) = 2\partial_\star \check{P}_i(2\mathbf{x} - \mathbf{1}), \quad \star \in \{x, y, z\}, \quad \mathbf{1} := (1, 1, 1)^\top.$$

5.2 Computing all quadrature nodes at once

Let Λ be the $N_{\text{qd}} \times 4$ matrix with the barycentric coordinates of the nodes of a quadrature formula (see Section 3.1). Let

$$\mathbf{X}^\mathcal{T}, \quad \mathbf{Y}^\mathcal{T}, \quad \mathbf{Z}^\mathcal{T}$$

be the $4 \times N_{\text{elt}}$ matrices with the (x, y, z) coordinates of the four vertices of all elements (we count elements by rows and vertices by columns). Then, the $N_{\text{qd}} \times N_{\text{elt}}$ matrices

$$\mathbf{X} := \Lambda \mathbf{X}^\mathcal{T}, \quad \mathbf{Y} := \Lambda \mathbf{Y}^\mathcal{T}, \quad \mathbf{Z} := \Lambda \mathbf{Z}^\mathcal{T}$$

contain the coordinates of all quadrature nodes on all the elements. Therefore, if f is a vectorized function of three variables, the $N_{\text{qd}} \times N_{\text{elt}}$ matrix $f(X, Y, Z)$ contains the values of f at all the quadrature nodes. The Matlab instruction to generate these points based on our data structure are:

```
x=T.coordinates(:,1); x=formula(:,[1 2 3 4])*x(T.elements');
y=T.coordinates(:,1); y=formula(:,[1 2 3 4])*y(T.elements');
z=T.coordinates(:,1); z=formula(:,[1 2 3 4])*z(T.elements');
```

5.3 Testing a function on elements

Given a vectorized function $f : \Omega \rightarrow \mathbb{R}$, we aim to compute the integrals

$$\int_K f P_i^K \quad i = 1, \dots, d_3, \quad K \in \mathcal{T}_h,$$

and store them in a $d_3 \times N_{\text{elt}}$ matrix. Let

$$P_{qj} := \hat{P}_j(\hat{\mathbf{p}}_q), \quad q = 1, \dots, N_{\text{qd}}, \quad j = 1, \dots, d_3.$$

Then

$$\int_K f P_i^K \approx |K| \sum_q \hat{\omega}_q f(\mathbf{p}_K^q) \hat{P}_i(\hat{\mathbf{p}}_q) = |K| \sum_q \hat{\omega}_q P_{qi} f(\mathbf{p}_K^q), \quad i = 1, \dots, d_3, \quad K \in \mathcal{T}_h.$$

If **vol** is the column vector with the volumes of all elements if $\hat{\omega}$ is the column vector with the weights of the quadrature rule, this formula is

$$\mathbf{vol}^\top \odot \left((\hat{\omega} \odot \mathbf{P})^\top f(X, Y, Z) \right).$$

Implementation notes. The code admits a row cell array of functions as input. If the array contains only one function, the output is a matrix. If the input contains several functions, then the output is a row cell array with the matrices.

```
function Ints=testElem(f,T,k,formula)

%{Int1,Int2,...}=testElem({f1,f2,...},T,k,formula)
%      Int=testElem({f},T,k,formula)
%
%Input:
% {f1,f2,...} : cell array with vectorized functions of three variables
%      T : expanded tetrahedrization
%      formula : 3d quadrature formula (Nnd x 5)
%      k : polynomial degree
%Output:
% {Int1,Int2,...}: each cell is d3 x Nelts (\int_K f{1} P_i^K)
%      Int : matrix \int_K f{1} P_i^K
%Last modified: March 14, 2013

x=T.coordinates(:,1);x=formula(:,1:4)*x(T.elements');
y=T.coordinates(:,2);y=formula(:,1:4)*y(T.elements');
z=T.coordinates(:,3);z=formula(:,1:4)*z(T.elements');
xhat=formula(:,2);
yhat=formula(:,3);
zhat=formula(:,4);

P=dubiner3d(2*xhat-1,2*yhat-1,2*zhat-1,k);
wP=bsxfun(@times,formula(:,5),P);

nInts=size(f,2);
```

```

if nInts==1
    Ints=bsxfun(@times,T.volume',wP'*f(x,y,z));
else
    Ints=cell(1,nInts);
    for n=1:nInts
        ff=f{n};
        Ints{n}=bsxfun(@times,T.volume',wP'*ff(x,y,z));
    end
end
return

```

5.4 Mass matrices

Given a vectorized function $m : \Omega \rightarrow \mathbb{R}$, we aim to compute the integrals

$$\int_K m P_i^K P_j^K \quad i, j = 1, \dots, d_3, \quad K \in \mathcal{T}_h,$$

and store them in a $d_3 \times d_3 \times N_{\text{elt}}$ array. We first change to the reference element and apply there a quadrature rule:

$$\int_K m P_i^K P_j^K \approx |K| \sum_q \hat{\omega}_q(\mathbf{p}_q^K) \hat{P}_i(\hat{\mathbf{p}}_q) \hat{P}_j(\hat{\mathbf{p}}_q).$$

Let X, Y, Z be the $N_{\text{qd}} \times N_{\text{elt}}$ matrices with the coordinates of all quadrature nodes and let \mathbf{vol} be the column vector with the volumes of the elements. We thus consider the $N_{\text{qd}} \times N_{\text{elt}}$ matrix

$$M = \mathbf{vol}^\top \odot m(X, Y, Z),$$

compute

$$\sum_q \mathbf{m}_q^\top \otimes (\hat{\omega}_q \mathbf{p}_q \mathbf{p}_q^\top), \quad \mathbf{m}_q^\top = \text{row}(M, q), \quad \mathbf{p}_q^\top = \text{row}(P, q),$$

and reshape this $d_3 \times (d_3 N_{\text{elt}})$ matrix as a $d_3 \times d_3 \times N_{\text{elt}}$ array.

Implementation notes. The code produces mass matrices associated to several coefficients. The input is a row cell array and the output a cell array whose elements are the mass matrices.

```

function Mass=MassMatrix(T,coeffs,k,formula)

%{M1,M2,...}=MassMatrix(T,{c1,c2,...},k,formula)
%Input:
%      T: expanded tetrahedrization
%      {c1,c2,...}: cell array with vectorized functions of three variables
%      k: polynomial degree
%      formula: quadrature formula in 3d (N x 5 matrix)
%
%Output:
% {M1,M2,...}: each cell is d3 x d3 x Nelts (\int_K c{1} P_i^K P_j^K )
%
%Last modified: March 14, 2013

Nnodes=size(formula,1);
Nelts=size(T.elements,1);
d3=nchoosek(k+3,3);

x=T.coordinates(:,1);x=formula(:,1:4)*x(T.elements');
y=T.coordinates(:,2);y=formula(:,1:4)*y(T.elements');
z=T.coordinates(:,3);z=formula(:,1:4)*z(T.elements'); % Nnd x Nelts
xhat=formula(:,2);
yhat=formula(:,3);

```

```

zhat=formula(:,4);

P=dubiner3d(2*xhat-1,2*yhat-1,2*zhat-1,k); % Nnd x d3

nMass=size(coeffs,2);
Mass=cell(1,nMass);
for n=1:nMass
    c=coeffs{n};
    C=bsxfun(@times,T.volume',c(x,y,z)); % Nnd x Nelts
    mass=zeros(d3,Nelts*d3);
    for q=1:Nnodes
        mass=mass+kron(C(q,:),formula(q,5)*P(q,:)'*P(q,:));
    end
    mass=reshape(mass,[d3,d3,Nelts]);
    Mass{n}=mass;
end
return

```

5.5 Convection matrices

The next aim is the computation of the matrices

$$\int_K P_i^K \partial_\star P_j^K, \quad i, j = 1, \dots, d_3, \quad K \in \mathcal{T}_h, \quad \star \in \{x, y, z\}$$

to be stored in $d_3 \times d_3 \times N_{\text{elt}}$ arrays C^\star . The first step will require the computation of matrices on the reference element by means of a quadrature formula of sufficiently high order:

$$\widehat{C}_{ij}^\star := \int_{\widehat{K}} \widehat{P}_i \partial_\star \widehat{P}_j = \frac{1}{6} \sum_q \widehat{\omega}_q \widehat{P}_i(\widehat{\mathbf{p}}_q) \partial_\star \widehat{P}_j(\widehat{\mathbf{p}}_q), \quad i, j = 1, \dots, d_3, \quad \star \in \{x, y, z\}.$$

If

$$P_{qi}^\star := \partial_\star \widehat{P}_i(\widehat{\mathbf{p}}_q), \quad q = 1, \dots, N_{\text{qd}}, \quad i = 1, \dots, d_3, \quad \star \in \{x, y, z\}$$

then

$$\widehat{C}^\star = \frac{1}{6} (\widehat{\omega} \odot P)^\top P^\star.$$

We next make a change of variables to the reference element

$$\begin{aligned} \int_K P_i^K \begin{bmatrix} \partial_x P_j^K \\ \partial_y P_j^K \\ \partial_z P_j^K \end{bmatrix} &= \det B_K \int_{\widehat{K}} \widehat{P}_i B_K^{-\top} \begin{bmatrix} \partial_x \widehat{P}_j^K \\ \partial_y \widehat{P}_j^K \\ \partial_z \widehat{P}_j^K \end{bmatrix} \\ &= \begin{bmatrix} a_{xx}^K & a_{xy}^K & a_{xz}^K \\ a_{yx}^K & a_{yy}^K & a_{yz}^K \\ a_{zx}^K & a_{zy}^K & a_{zz}^K \end{bmatrix} \begin{bmatrix} \widehat{C}_{ij}^x \\ \widehat{C}_{ij}^y \\ \widehat{C}_{ij}^z \end{bmatrix}, \quad \det B_K B_K^{-\top} = \begin{bmatrix} a_{xx}^K & a_{xy}^K & a_{xz}^K \\ a_{yx}^K & a_{yy}^K & a_{yz}^K \\ a_{zx}^K & a_{zy}^K & a_{zz}^K \end{bmatrix}, \end{aligned}$$

with (the element index K is omitted)

$$\begin{aligned}
a_{xx} &= (y_3 - y_1)(z_4 - z_1) - (y_4 - y_1)(z_3 - z_1), \\
a_{xy} &= (y_4 - y_1)(z_2 - z_1) - (y_2 - y_1)(z_4 - z_1), \\
a_{xz} &= (y_2 - y_1)(z_3 - z_1) - (y_3 - y_1)(z_2 - z_1), \\
a_{yx} &= (x_4 - x_1)(z_3 - z_1) - (x_3 - x_1)(z_4 - z_1), \\
a_{yy} &= (x_2 - x_1)(z_4 - z_1) - (x_4 - x_1)(z_2 - z_1), \\
a_{yz} &= (x_3 - x_1)(z_2 - z_1) - (x_2 - x_1)(z_3 - z_1), \\
a_{zx} &= (x_3 - x_1)(y_4 - y_1) - (x_4 - x_1)(y_3 - y_1), \\
a_{zy} &= (x_4 - x_1)(y_2 - y_1) - (x_2 - x_1)(y_4 - y_1), \\
a_{zz} &= (x_2 - x_1)(y_3 - y_1) - (x_3 - x_1)(y_2 - y_1).
\end{aligned}$$

If the previous nine quantities are computed for each of the elements and stored in nine *column* vectors with N_{elt} components, it follows that

$$\begin{aligned}
C^x &= \mathbf{a}_{xx}^\top \otimes \hat{C}^x + \mathbf{a}_{xy}^\top \otimes \hat{C}^y + \mathbf{a}_{xz}^\top \otimes \hat{C}^z, \\
C^y &= \mathbf{a}_{yx}^\top \otimes \hat{C}^x + \mathbf{a}_{yy}^\top \otimes \hat{C}^y + \mathbf{a}_{yz}^\top \otimes \hat{C}^z, \\
C^z &= \mathbf{a}_{zx}^\top \otimes \hat{C}^x + \mathbf{a}_{zy}^\top \otimes \hat{C}^y + \mathbf{a}_{zz}^\top \otimes \hat{C}^z,
\end{aligned}$$

that is

$$C^* = \sum_{\# \in \{x,y,z\}} \mathbf{a}_{*\#}^\top \otimes \hat{C}^\#.$$

```

function [convx,convy,convz]=ConvMatrix(T,k,formula)

%[convx,convy,convz]=ConvMatrix(T,k,formula)
%
%Input:
%      T: expanded tetrahedrization
%      k: polynomial degree
%      formula: quadrature formula in 3d (N x 5 matrix)
%
%Output:
%      convx: d3 x d3 x Nelts ( \int_K P_i^K \partial_x P_j^K )
%      convy: d3 x d3 x Nelts ( \int_K P_i^K \partial_y P_j^K )
%      convz: d3 x d3 x Nelts ( \int_K P_i^K \partial_z P_j^K )
%
%Last modified: March 14, 2013

Nelts=size(T.elements,1);
d3=nchoosek(k+3,3);

xhat=formula(:,2);
yhat=formula(:,3);
zhat=formula(:,4);

[p,px,py,pz]=dubiner3d(2*xhat-1,2*yhat-1,2*zhat-1,k);
px=2*px;
py=2*py;
pz=2*pz;
wp=bsxfun(@times,formula(:,5),p);

convhatx=1/6*wp'*px;
convhaty=1/6*wp'*py;
convhatz=1/6*wp'*pz;

```

```

x12=T.coordinates(T.elements(:,2),1)-T.coordinates(T.elements(:,1),1); %x2-x1
x13=T.coordinates(T.elements(:,3),1)-T.coordinates(T.elements(:,1),1); %x3-x1
x14=T.coordinates(T.elements(:,4),1)-T.coordinates(T.elements(:,1),1); %x4-x1
y12=T.coordinates(T.elements(:,2),2)-T.coordinates(T.elements(:,1),2); %y2-y1
y13=T.coordinates(T.elements(:,3),2)-T.coordinates(T.elements(:,1),2); %y3-y1
y14=T.coordinates(T.elements(:,4),2)-T.coordinates(T.elements(:,1),2); %y4-y1
z12=T.coordinates(T.elements(:,2),3)-T.coordinates(T.elements(:,1),3); %z2-z1
z13=T.coordinates(T.elements(:,3),3)-T.coordinates(T.elements(:,1),3); %z3-z1
z14=T.coordinates(T.elements(:,4),3)-T.coordinates(T.elements(:,1),3); %z4-z1

axx=y13.*z14-y14.*z13;
axy=y14.*z12-y12.*z14;
axz=y12.*z13-y13.*z12;
ayx=x14.*z13-x13.*z14;
ayy=x12.*z14-x14.*z12;
ayz=x13.*z12-x12.*z13;
azx=x13.*y14-x14.*y13;
azy=x14.*y12-x12.*y14;
azz=x12.*y13-x13.*y12;

convx=kron(axx',convhatx)+kron(axy',convhaty)+kron(axz',convhatz);
convy=kron(ayx',convhatx)+kron(ayy',convhaty)+kron(ayz',convhatz);
convz=kron(azx',convhatx)+kron(azy',convhaty)+kron(azz',convhatz);

convx=reshape(convx,[d3,d3,Nelts]);
convy=reshape(convy,[d3,d3,Nelts]);
convz=reshape(convz,[d3,d3,Nelts]);
return

```

5.6 A function for errors

Given a function $u : \Omega \rightarrow \mathbb{R}$ and a piecewise polynomial function $u_h \in W_h$, the aim of this part is the approximated computation of

$$\left(\sum_{K \in \mathcal{T}_h} |u - u_h|^2 \right)^{1/2}.$$

As usual, let X, Y, Z be the $N_{qd} \times N_{elt}$ matrices with the coordinates of the quadrature nodes on all the elements and let

$$P_{qi} := \hat{P}_i(\hat{\mathbf{p}}_q) \quad q = 1, \dots, N_{qd}, \quad i = 1, \dots, d_3.$$

Assuming that the coefficients of u_h are given in a $d_3 \times N_{elt}$ matrix U , it follows that PU are the values of u_h on all quadrature nodes, and therefore the $N_{qd} \times N_{elt}$ matrix

$$E := PU - u(X, Y, Z) \quad E_{qK} := u_h(\mathbf{p}_q^K) - u(\mathbf{p}_q^K)$$

contains the differences at all quadrature points. The computation of the error is just a vector-matrix-vector multiplication, after element-by-element squaring the values E_{qK} :

$$\left(\sum_{q,K} \hat{\omega}_q E_{qK}^2 |K| \right)^{1/2}.$$

```

function error=errorElem(T,p,ph,k,formula)

%error=errorElem(T,p,ph,k,formula)
%
%Input:
%      T: expanded tetrahedrization
%      p: vectorized function of three variables

```

```

%           ph: discontinuous Pk function (d3 x Nelts)
%           k: polynomial degree
%           formula: quadrature formula in 3d (N x 5 matrix)
%
%Output:
%           error: || p - ph ||_{L^2}
%
%Last modified: May 31, 2012

x=T.coordinates(:,1); x=formula(:,1:4)*x(T.elements');
y=T.coordinates(:,2); y=formula(:,1:4)*y(T.elements');
z=T.coordinates(:,3); z=formula(:,1:4)*z(T.elements');
p=p(x,y,z);

xhat=formula(:,2);
yhat=formula(:,3);
zhat=formula(:,4);
B=dubiner3d(2*xhat-1,2*yhat-1,2*zhat-1,k);
ph=B*ph;

error=sqrt(formula(:,5)'*(p-ph).^2*T.volume);
return

```

6 Surface matrices and integrals

6.1 Piecewise polynomial functions on the skeleton

Given a face $e \in \mathcal{E}_h$, a basis for $\mathcal{P}_k(e)$ is defined by pushing forward the basis on \widehat{K}_2 using the parametrization ϕ_e , namely,

$$D_i^e \circ \phi_e = \widehat{D}_i, \quad i = 1, \dots, d_2, \quad e \in \mathcal{E}_h.$$

The skeleton of the triangulation $\partial\mathcal{T}_h$ is the set formed by joining all faces of all elements. A function in the space

$$M_h := \prod_{e \in \mathcal{E}_h} \mathcal{P}_k(e) = \{\widehat{u}_h : \partial\mathcal{T}_h \rightarrow \Omega : \widehat{u}_h|_e \in \mathcal{P}_k(e) \quad \forall e \in \mathcal{E}_h\}, \quad \partial\mathcal{T}_h = \bigcup_{e \in \mathcal{E}_h} e,$$

can be stored in two ways: as a $d_2 \times N_{\text{fc}}$ matrix, whose e -th column stores the coefficients of the function on the face e , or as a $d_2 N_{\text{fc}}$ column vector, with blocks of d_2 elements corresponding to the faces.

Warning. Similarly to what we do in $\mathcal{P}_k(\widehat{K})$, for two dimensional functions we will be using a Dubiner basis, that is orthogonal in $\check{K}_2 := 2\widehat{K}_2 - \mathbf{1}$. Therefore, at each evaluation of basis functions we have to apply the substitution

$$\widehat{D}_i(\mathbf{x}) = \check{D}_i(2\mathbf{x} - \mathbf{1}).$$

6.2 Testing on faces

Let $f : \Omega \rightarrow \mathbb{R}$. The aim of this function is the approximation of

$$\int_e f D_i^e \quad i = 1, \dots, d_2, \quad e \in \mathcal{E}_h,$$

which will be stored as a $d_2 \times N_{\text{fc}}$ matrix. This process is very similar to the one explained in Section 5.3 for testing on elements. We first write the approximations in the form

$$\int_e f D_i^e \approx |e| \sum_r \varpi_r \widehat{D}_i(\widehat{\mathbf{q}}_r) f(\mathbf{q}_r^e), \quad \text{where} \quad \mathbf{q}_r^e = \phi_e(\widehat{\mathbf{q}}_r).$$

To evaluate f at all quadrature points, we start by constructing three $3 \times N_{fc}$ matrices $X^{\mathcal{E}}$, $Y^{\mathcal{E}}$, and $Z^{\mathcal{E}}$, with the respective coordinates of the three vertices of each of the faces. If Ξ is the $N_{qd2} \times 3$ matrix with the barycentric coordinates of all quadrature points (the first three columns of the matrix where we store the quadrature formula), then

$$X = \Xi X^{\mathcal{E}}, \quad Y = \Xi Y^{\mathcal{E}}, \quad Z = \Xi Z^{\mathcal{E}}$$

are $N_{qd2} \times N_{fc}$ matrices with the coordinates of all quadrature points on the faces, as mapped from the reference element with the intrinsic parametrization of each element. With the given data structure, this construction is easily accomplished. For instance:

```
x=T.coordinates(:,1); x=formula(:,1:3)*x(T.faces(:,1:3)');

```

(Recall that the last column of **T.faces** contains information about the location of the face in the interior domain, Dirichlet boundary or Neumann boundary.) If

$$D_{rj} = \hat{D}_j(\hat{\mathbf{q}}_r), \quad r = 1, \dots, N_{qd}, \quad j = 1, \dots, d_2,$$

ϖ is the column vector with the weights of the quadrature formula, and **area** is the column vector with the areas of the elements, then the result is just

$$\mathbf{area} \odot \left((\varpi \odot D)^{\top} f(X, Y, Z) \right),$$

reshaped as a three dimensional array.

Implementation notes. For input/output, see `testElem.m` in Section 5.3

```
function Ints=testFaces(f,T,k,formula)

%{Int1,Int2,...}=testFaces({f1,f2,...},T,k,formula)
%   Int=testFaces({f1},T,k,formula)
%
%Input:
% {f1,f2,...}: each cell is a vectorized function of three variables
%   T: expanded tetrahedrization
%   formula: quadrature formula in 2d (N x 4 matrix)
%   k: polynomial
%
%Output:
% {Int1,Ints2,...}: each cell is a d2 x Nfaces matrix
%   ( \int_e f{1} D_i^e )
%
%Last modified: March 14, 2013

x=T.coordinates(:,1); x=formula(:,1:3)*x(T.faces(:,[1 2 3]))';
y=T.coordinates(:,2); y=formula(:,1:3)*y(T.faces(:,[1 2 3]))';
z=T.coordinates(:,3); z=formula(:,1:3)*z(T.faces(:,[1 2 3]))';

DB=dubiner2d(2*formula(:,2)-1,2*formula(:,3)-1,k);
DB=bsxfun(@times,formula(:,4),DB);

nInts=size(f,2);
if nInts==1
    Ints=bsxfun(@times,T.area',DB'*f(x,y,z));
else
    Ints=cell(1,nInts);
    for n=1:nInts
        ff=f{n};
        Ints{n}=bsxfun(@times,T.area',DB'*ff(x,y,z));
    end
end
return

```

6.3 The penalization parameter τ

Piecewise constant functions on the boundaries of the elements,

$$\xi \in \mathcal{P}_0(\partial\mathcal{T}_h) := \prod_{K \in \mathcal{T}_h} \prod_{e \in \mathcal{E}(K)} \mathcal{P}_0(e),$$

will be stored as $4 \times N_{\text{elt}}$ matrices and denoted ξ_ℓ^K . These functions can be double valued on internal faces. Some simple but relevant piecewise constant functions, that can be taken from geometric information, are

```
T.area(T.facebyele')
nx=T.normals(:, [1 4 7 10])';
ny=T.normals(:, [2 5 8 11])';
nz=T.normals(:, [3 6 9 12])';
```

The first one has been denoted so far e_ℓ^K . The one with components of the normal vectors will be denoted $n_\star \in \mathcal{P}_0(\partial\mathcal{T}_h)$, for $\star \in \{x, y, z\}$.

An important part of the HDG scheme is a penalization function $\tau \in \mathcal{P}_0(\partial\mathcal{T}_h)$. Currently, the code supports three choices: constant $\tau \equiv 1$, the first face choice

$$\tau_1^K = 1, \quad K \in \mathcal{T}_h, \quad \text{and} \quad \tau_\ell^K = 0, \quad \ell \in \{2, 3, 4\}, \quad K \in \mathcal{T}_h,$$

and the one random face choice (using a discrete uniform random distribution to choose one face on each element)

$$\tau_\ell^K = \delta_{\ell(K)}^K \quad \ell(K) \in \{1, 2, 3, 4\}.$$

```
function tau=createTau3d(Nelts,option)

% tau=createTau3d(Nelts,option)
%
% Input:
%   Nelts    : number of elements
%   option    : (1) tau = 1
%               (2) SFHDG on the first face
%               (3) SFHDG on a random face
% Output:
%   tau       : 4 x Nelts
%
% Last modified: March 14, 2013

switch option
case 1
    tau=ones(4,Nelts);
case 2
    tau=[ones(1,Nelts);...
         zeros(3,Nelts)];
case 3
    where=ceil(4*rand(1,Nelts));
    tau=sparse(where,1:Nelts,1);
    tau=full(tau);
end
return
```

6.4 Three types of surface matrices

Type (a)

The aim of this section is the computation of

$$\int_{\partial K} P_i^K P_j^K \quad i, j = 1, \dots, d_3, \quad K \in \mathcal{T}_h,$$

and its storage as a $d_3 \times d_3 \times N_{\text{elt}}$ array. Using a quadrature formula of sufficiently high order, we can write

$$\int_{\partial K} P_i^K P_j^K = \sum_{\ell=1}^4 \tau_\ell^K |e_\ell^K| \sum_r \hat{P}_i(\hat{\mathbf{q}}_r^\ell) \varpi_r \hat{P}_j(\hat{\mathbf{q}}_r^\ell).$$

We first compute four $N_{\text{qd}} \times d_3$ matrices

$$\mathbf{P}_{ri}^\ell = \hat{P}_i(\hat{\mathbf{q}}_r^\ell), \quad r = 1, \dots, N_{\text{qd}2}, \quad i = 1, \dots, d_3, \quad \ell \in \{1, 2, 3, 4\},$$

and then

$$\sum_{\ell=1}^4 \mathbf{t}_\ell^\top \otimes \left((\boldsymbol{\varpi} \odot \mathbf{P}^\ell)^\top \mathbf{P}^\ell \right), \quad \mathbf{t}_\ell^\top = \text{row}(\mathbf{T}, \ell), \quad \mathbf{T}_K^\ell := \tau_K^\ell |e_\ell^K|.$$

The result is a $d_3 \times (d_3 N_{\text{elt}})$ matrix that is then reshaped as a $d_3 \times d_3 \times N_{\text{elt}}$ array.

Type (b)

The second group of matrices is

$$\tau_\ell^K \int_{e_\ell^K} D_i^{e_\ell^K} D_j^{e_\ell^K} \quad \begin{array}{l} i = 1, \dots, d_2 \\ j = 1, \dots, d_3 \end{array} \quad \begin{array}{l} K \in \mathcal{T}_h \\ \ell \in \{1, 2, 3, 4\}, \end{array}$$

to be stored as the diagonal blocks of a block-diagonal $4d_2 \times 4d_2 \times N_{\text{elt}}$ array. Using quadrature and the fact that we are free to choose the parametrization ϕ_e when $e = e_\ell^K$, we arrive at

$$\int_{e_\ell^K} \tau D_i^{e_\ell^K} D_j^{e_\ell^K} = |e_\ell^K| \tau_\ell^K \sum_r \varpi_r \hat{D}_i(\hat{\mathbf{q}}_r) \hat{D}_j(\hat{\mathbf{q}}_r),$$

so the ℓ -th block is

$$\mathbf{t}_\ell^\top \otimes \left((\boldsymbol{\varpi} \odot \mathbf{P})^\top \mathbf{P} \right).$$

Type (c)

The third group of boundary matrices produces (simultaneously) matrices

$$\frac{\xi_K^\ell}{|e_\ell^K|} \int_{e_\ell^K} D_i^{e_\ell^K} P_i^K, \quad \begin{array}{l} i = 1, \dots, d_2 \\ j = 1, \dots, d_3 \end{array} \quad \begin{array}{l} K \in \mathcal{T}_h \\ \ell \in \{1, 2, 3, 4\} \end{array}$$

that will be stored as $4d_2 \times d_3 \times N_{\text{elt}}$ arrays, in blocks of $d_2 \times d_3 \times N_{\text{elt}}$ arrays corresponding to the four values of ℓ . Here ξ is a piecewise constant function. In practice we need

$$\xi_\ell^K = \mathbf{T}_\ell^K = \tau_\ell^K |e_\ell^K|, \quad \xi_\ell^K = n_{\ell, \star}^K \quad \star \in \{x, y, z\},$$

where $n_{\ell, \star}^K$ is the \star component of the non-normalized outward normal vector on e_ℓ^K . Using the notation of Section 3.3 and a quadrature formula of sufficiently high order, the integrals are then

$$\begin{aligned} \frac{\xi_K^\ell}{|e_\ell^K|} \int_{e_\ell^K} D_i^{e_\ell^K} P_i^K &= \xi_\ell^K \sum_r \hat{D}_i(F_{\text{perm}(K, \ell)}(\hat{\mathbf{q}}_r)) \varpi_r \hat{P}_j(\hat{\mathbf{q}}_r^\ell) \\ &= \sum_{\mu=1}^6 \xi_\ell^K \mathbf{1}_{\text{perm}(K, \ell)=\mu} \left(\sum_r \hat{D}_i(F_\mu(\hat{\mathbf{q}}_r)) \varpi_r \hat{P}_j(\hat{\mathbf{q}}_r^\ell) \right) \end{aligned}$$

Let then $\xi_\mu \in \mathcal{P}_0(\partial \mathcal{T}_h)$ be given by

$$\xi_{\ell, \mu}^K = \xi_\ell^K \mathbf{1}_{\text{perm}(K, \ell)=\mu} = \begin{cases} \xi_\ell^K & \text{if } \text{perm}(K, \ell) = \mu, \\ 0, & \text{otherwise.} \end{cases}$$

Then, we just need to compute

$$\sum_{\mu=1}^6 \boldsymbol{\xi}_{\ell, \mu}^\top \otimes ((\boldsymbol{\varpi} \odot \mathbf{D}^\mu)^\top \mathbf{P}^\ell), \quad \boldsymbol{\xi}_{\ell, \mu}^\top = \text{row}(\boldsymbol{\xi}_\mu, \ell),$$

where

$$\begin{aligned} \mathbf{P}_{ri}^\ell &= \widehat{P}_i(\widehat{\mathbf{q}}_r^\ell), & r = 1, \dots, N_{\text{qd}2}, & \quad i = 1, \dots, d_3, \\ \mathbf{D}_{ri}^\mu &= \widehat{D}_i(F_\mu(\widehat{\mathbf{q}}_r)), & r = 1, \dots, N_{\text{qd}2}, & \quad i = 1, \dots, d_2. \end{aligned}$$

Implementation notes. The matrices $(\varpi \odot D^\mu)^\top P^\ell$ are stored in a single $6d_2 \times 4d_3$ array. Two local anonymous functions are defined for easy access to local degrees of freedom. The `block2` and `block3` functions produce the lists

$$(\ell - 1)d_2 + \{1, 2, \dots, d_2\} \quad \text{and} \quad (\ell - 1)d_3 + \{1, 2, \dots, d_3\}$$

respectively. These lists allow for easy location of blocks in the $6d_2 \times 4d_3$ array that stores them.

```

function [tauPP,tauDP,nxDP,nyDP,nzDP,tauDD]=matricesFace(T,tau,k,formula)
%
%[tauPP,tauDP,nxDP,nyDP,nzDP,tauDD]=matricesFace(T,tau,k,formula)
%
%Input:
%      T: expanded terahedrization
%      tau: penalization parameter for HDG (Nelts x 4)
%      k: polynomial degree
%      formula: quadrature formula in 2d (N x 4 matrix)
%Output:
%      tauPP : d3 x d3 x Nelts, with <tau P_{i,j}>_{-{\partial K}}
%      tauDP : 4*d2 x d3 x Nelts, with <tau D_{i,j}>_{-e, e \in E(K)}
%      nxDP : 4*d2 x d3 x Nelts, with <n_x D_{i,j}>_{-e, e \in E(K)}
%      nyDP : 4*d2 x d3 x Nelts, with <n_y D_{i,j}>_{-e, e \in E(K)}
%      nzDP : 4*d2 x d3 x Nelts, with <n_z D_{i,j}>_{-e, e \in E(K)}
%      tauDD : 4*d2 x 4*d2 x Nelts, block diag <tau D_{i,j}>_{-e, e \in E(K)}
%
%Last modified: March 14, 2013

Nelts=size(T.elements,1);
Nnodes=size(formula,1);
TauArea=T.area(T.facebyele').*tau; % 4 x Nelts
T.perm=T.perm'; % 4 x Nelts

d2=nchoosek(k+2,2);
d3=nchoosek(k+3,3);

s=formula(:,2);
t=formula(:,3);
weights=formula(:,4);

% Computation <tau*Pi,Pj>

O=zeros(size(s));
points3d=[s,t,O;...
          s,O,t;...
          O,s,t;...
          s,t,1-s-t];

pb=dubiner3d(2*points3d(:,1)-1,2*points3d(:,2)-1,2*points3d(:,3)-1,k); %4*Nnodes x d3
pbweights=bsxfun(@times,[formula(:,4);...
                        formula(:,4);...
                        formula(:,4);...

```

```

        formula(:,4)],pb);
pbpb1=pbweights(1:Nnodes,:)'*pb(1:Nnodes,:);
pbpb2=pbweights(Nnodes+1:2*Nnodes,:)'*pb(Nnodes+1:2*Nnodes,:);
pbpb3=pbweights(2*Nnodes+1:3*Nnodes,:)'*pb(2*Nnodes+1:3*Nnodes,:);
pbpb4=pbweights(3*Nnodes+1:4*Nnodes,:)'*pb(3*Nnodes+1:4*Nnodes,:);

tauPP=kron(TauArea(1,:),pbpb1)+kron(TauArea(2,:),pbpb2)...
+kron(TauArea(3,:),pbpb3)+kron(TauArea(4,:),pbpb4);
tauPP=reshape(tauPP,[d3,d3,Nelts]);

% Computation <alpha*D,P>, alpha=tau,nx,ny,nz,

pb=[pb(1:Nnodes,:),pb(Nnodes+1:2*Nnodes,:),...
pb(2*Nnodes+1:3*Nnodes,:),pb(3*Nnodes+1:4*Nnodes,:)]'; % Nnodes x 4*d3
points2d=[s,t;...
t,s;...
1-s-t,s;...
s,1-s-t;...
t,1-s-t;...
1-s-t,t];
db=dubiner2d(2*points2d(:,1)-1,2*points2d(:,2)-1,k); % 6*Nnodes x d2
db=[db(1:Nnodes,:),db(Nnodes+1:2*Nnodes,:),...
db(2*Nnodes+1:3*Nnodes,:),db(3*Nnodes+1:4*Nnodes,:),...
db(4*Nnodes+1:5*Nnodes,:),db(5*Nnodes+1:6*Nnodes,:)]'; % Nnodes x 6*d2
db=bsxfun(@times,weights,db);
allproducts=db'*pb; %6*d2 x 4*d3

block2=@(x) (1+(x-1)*d2):(x*d2);
block3=@(x) (1+(x-1)*d3):(x*d3);

tauDP=zeros(4*d2,d3*Nelts);
nxDP=zeros(4*d2,d3*Nelts);
nyDP=zeros(4*d2,d3*Nelts);
nzDP=zeros(4*d2,d3*Nelts);
for l=1:4
    Nx=T.normals(:,3*(l-1)+1)';
    Ny=T.normals(:,3*(l-1)+2)';
    Nz=T.normals(:,3*(l-1)+3)';
    for mu=1:6
        taumu=TauArea(l,:).*(T.perm(l,')==mu);
        tauDP(block2(1),:)=tauDP(block2(1),:)+...
            kron(taummu,allproducts(block2(mu),block3(1)));

        nxmu=Nx.*(T.perm(l,')==mu);
        nxDP(block2(1),:)=nxDP(block2(1),:)+...
            kron(nxmu,allproducts(block2(mu),block3(1)));

        nymu=Ny.*(T.perm(l,')==mu);
        nyDP(block2(1),:)=nyDP(block2(1),:)+...
            kron(nymu,allproducts(block2(mu),block3(1)));

        nzmu=Nz.*(T.perm(l,')==mu);
        nzDP(block2(1),:)=nzDP(block2(1),:)+...
            kron(nzmu,allproducts(block2(mu),block3(1)));
    end
end
tauDP=reshape(tauDP,[4*d2,d3,Nelts]);
nxDP=reshape(nxDP,[4*d2,d3,Nelts]);
nyDP=reshape(nyDP,[4*d2,d3,Nelts]);
nzDP=reshape(nzDP,[4*d2,d3,Nelts]);

% Computation tauDD

d=dubiner2d(2*s-1,2*t-1,k);
dweights=bsxfun(@times,d,weights);
dwd=dweights'*d;

```

```

tauDD=zeros(4*d2,4*d2,Nelts);
for l=1:4
    tauDD(block2(l),block2(l),:)=reshape(kron(TauArea(l,:),dwd),...
                                           [d2,d2,Nelts]);
end
return

```

6.5 Another function for errors

Given $u : \Omega \rightarrow \mathbb{R}$ and $\hat{u}_h \in M_h$ (stored as a $d_2 \times N_{fc}$ matrix), we want to compute

$$\|\hat{u}_h - u\|_h := \left(\sum_{e \in \mathcal{E}_h} |e| \int_e |\hat{u}_h - u|^2 \right)^{1/2}.$$

Note that

$$\sum_{e \in \mathcal{E}_h} |e| \int_e |\hat{u}_h - u|^2 \approx \sum_{e \in \mathcal{E}_h} \sum_r \varpi_r |\hat{u}_h(\mathbf{q}_r^e) - u(\mathbf{q}_r^e)|^2 |e|^2.$$

What is left is very similar to what was done in Section 5.6 to compute L^2 errors. We start computing three $N_{qd2} \times N_{fc}$ matrices X, Y, Z , with the coordinates of all quadrature nodes \mathbf{q}_r^e , and the $N_{qd2} \times d_2$ matrix

$$D_{ri} := \hat{D}_i(\hat{\mathbf{q}}_r) \quad r = 1, \dots, N_{qd2}, \quad i = 1, \dots, d_2.$$

If U is the $d_2 \times N_{fc}$ matrix with the coefficients of \hat{u}_h , then

$$E := DU - u(X, Y, Z) \quad E_{re} := \hat{u}_h(\mathbf{q}_r^e) - u(\mathbf{q}_r^e)$$

are the pointwise errors and the total error is just

$$\left(\sum_{r,e} \varpi_r E_{re}^2 |e|^2 \right)^{1/2}.$$

```

function error=errorFaces(T,p,ph,k,formula)

%error =errorFaces(T,p,ph,k,formula)
%
%Input:
%      T: expanded tetrahedrization
%      p: vectorized function of three variables
%      ph: Pk function on skeleton (d2 x Nfaces)
%      k: polynomial degree
%      formula: quadrature formula in 2d (N x 4 matrix)
%
%Output:
%      error: || p - ph ||_{h,\partial T}
%
%Last modified: March 14, 2013

x=T.coordinates(:,1);x=formula(:,[1 2 3])*x(T.faces(:,[1 2 3]))';
y=T.coordinates(:,2);y=formula(:,[1 2 3])*y(T.faces(:,[1 2 3]))';
z=T.coordinates(:,3);z=formula(:,[1 2 3])*z(T.faces(:,[1 2 3]))';
p=p(x,y,z); %Nnodes x Nfaces

DB=dubiner2d(2*formula(:,2)-1,2*formula(:,3)-1,k);
ph=DB*ph; %Nnodes x Nfaces

error=sqrt(formula(:,4)'+(p-ph).^2*(T.area).^2);
return

```

7 Local solvers

The local solvers that we next defined are related to the pair of first order PDEs

$$\kappa^{-1} \mathbf{q} + \nabla u = 0, \quad \text{and} \quad \nabla \cdot \mathbf{q} + cu = f \quad \text{in } \Omega.$$

7.1 Matrices and bilinear forms

In order to recognize the matrices that we have computed with terms in the bilinear forms of the HDG method, we need some notation. We will write

$$(u, v)_K := \int_K u v, \quad \langle u, v \rangle_{\partial K} := \int_{\partial K} u v$$

and we will consider the space

$$\mathcal{R}_k(\partial K) := \prod_{e \in \mathcal{E}(K)} \mathcal{P}_k(e), \quad \dim \mathcal{R}_k(\partial K) = 4d_2.$$

The degrees of freedom for this last space are organized by taking one face at a time in the order they are given by `T.facebyele`.

For (non-symmetric) bilinear forms we will use the convention that the bilinear form $b(u, v)$ is related to the matrix $b(U_j, V_i)$, where $\{U_j\}$ is a basis of the space of u and $\{V_i\}$ is a basis of the space for v . This is equivalent to saying that the unknown will always be placed as the left-most argument in the bilinear form and the test function will occupy the right-most location.

Volume terms. We start by computing mass matrices associated to two functions (κ^{-1} and c), and the three convection matrices:

$$\mathbf{M}_{\kappa^{-1}}^K, \quad \mathbf{M}_c^K, \quad \mathbf{C}_x^K, \quad \mathbf{C}_y^K, \quad \mathbf{C}_z^K,$$

where

$$(\mathbf{M}_m^K)_{ij} = \int_K m P_i^K P_j^K, \quad (\mathbf{C}_\star^K)_{ij} = \int_K P_i^K \partial_\star P_j^K.$$

Each of these matrices is $d_3 \times d_3 \times N_{\text{elt}}$. They correspond to the bilinear forms

$$(m u_h, v_h)_K \quad (\partial_\star u_h, v_h)_K \quad u_h, v_h \in \mathcal{P}_k(K).$$

Surface terms. We next compute all matrices related to integrals on interfaces:

$$\tau \mathbf{PP}^K, \quad \tau \mathbf{DP}^K, \quad n_x \mathbf{DP}^K, \quad n_y \mathbf{DP}^K, \quad n_z \mathbf{DP}^K, \quad \tau \mathbf{DD}^K.$$

The first of these arrays is $d_3 \times d_3 \times N_{\text{elt}}$, the next four are $4d_2 \times d_3 \times N_{\text{elt}}$ and the last one is $4d_2 \times 4d_2 \times N_{\text{elt}}$. The first matrix and associated bilinear form is

$$\tau \mathbf{PP}_{ij}^K = \int_{\partial K} \tau P_i^K P_j^K, \quad \langle \tau u_h, v_h \rangle_{\partial K} \quad u_h, v_h \in \mathcal{P}_k(K).$$

The second one corresponds to the bilinear forms

$$\langle \tau u_h, \hat{v}_h \rangle_{\partial K} \quad u_h \in \mathcal{P}_k(K), \quad \hat{v}_h \in \mathcal{R}_k(\partial K)$$

or equivalently to

$$\langle \tau u_h, \hat{v}_h \rangle_e \quad u_h \in \mathcal{P}_k(K), \quad \hat{v}_h \in \mathcal{P}_k(e), \quad e \in \mathcal{E}(K).$$

The matrices associated to the components of the normal vector $\boldsymbol{\nu} = (\nu_x, \nu_y, \nu_z)$ are related to the bilinear forms

$$\langle \nu_\star u_h, \hat{v}_h \rangle_{\partial K} \quad u_h \in \mathcal{P}_k(K), \quad \hat{v}_h \in \mathcal{R}_k(\partial K), \quad \star \in \{x, y, z\}.$$

The last matrix corresponds to

$$\langle \tau \hat{u}_h, \hat{v}_h \rangle_{\partial K} \quad \hat{u}_h, \hat{v}_h \in \mathcal{R}_k(\partial K)$$

and is therefore block diagonal.

Finally we compute the vectors of tests of f with the basis elements of $\mathcal{P}_k(K)$: $\mathbf{f}^K \in \mathbb{R}^{d_3}$.

7.2 Matrices related to local solvers

The $4d_3 \times 4d_3 \times N_{\text{elt}}$ array with slices

$$\mathbb{A}_1^K := \begin{bmatrix} M_{\kappa^{-1}}^K & \mathbf{O} & \mathbf{O} & -(\mathbf{C}_x^K)^\top \\ \mathbf{O} & M_{\kappa^{-1}}^K & \mathbf{O} & -(\mathbf{C}_y^K)^\top \\ \mathbf{O} & \mathbf{O} & M_{\kappa^{-1}}^K & -(\mathbf{C}_z^K)^\top \\ \mathbf{C}_x^K & \mathbf{C}_y^K & \mathbf{C}_z^K & M_c^K + \tau \mathbf{P} \mathbf{P}^K \end{bmatrix},$$

is the matrix representation of the bilinear form $(\mathcal{P}_k(K)^3 \times \mathcal{P}_k(K)) \times (\mathcal{P}_k(K)^3 \times \mathcal{P}_k(K)) \rightarrow \mathbb{R}$:

$$\begin{aligned} (\mathbf{q}_h, u_h) \quad , \quad (\mathbf{r}_h, w_h) \quad \longmapsto \quad & (\kappa^{-1} \mathbf{q}_h, \mathbf{r}_h)_K - (u_h, \nabla \cdot \mathbf{r}_h)_K \\ & + (\nabla \cdot \mathbf{q}_h, w_h)_K + (c u_h, w_h)_K + \langle \tau u_h, v_h \rangle_{\partial K} \end{aligned}$$

The $4d_3 \times 4d_2 \times N_{\text{elt}}$ array with slices

$$\mathbb{A}_2^K := \begin{bmatrix} (n_x \mathbf{D} \mathbf{P}^K)^\top \\ (n_y \mathbf{D} \mathbf{P}^K)^\top \\ (n_z \mathbf{D} \mathbf{P}^K)^\top \\ -(\tau \mathbf{D} \mathbf{P}^K)^\top \end{bmatrix}$$

is the matrix representation of the bilinear form $\mathcal{R}_k(\partial K) \times (\mathcal{P}_k(K)^3 \times \mathcal{P}_k(K)) \rightarrow \mathbb{R}$:

$$\hat{u}_h \quad , \quad (\mathbf{r}_h, w_h) \quad \longmapsto \quad \langle \hat{u}_h, \mathbf{r}_h \cdot \boldsymbol{\nu} \rangle_{\partial K} - \langle \tau \hat{u}_h, w_h \rangle_{\partial K}.$$

If $\hat{u}_h \in M_h$ is known, we can solve the local problems looking for $\mathbf{q}_h \in \mathbf{V}_h := W_h^3$ and $u_h \in W_h$ such that

$$\begin{aligned} (\kappa^{-1} \mathbf{q}_h, \mathbf{r}_h)_K - (u_h, \nabla \cdot \mathbf{r}_h)_K + \langle \hat{u}_h, \mathbf{r}_h \cdot \boldsymbol{\nu} \rangle_{\partial K} &= 0 \quad \forall \mathbf{r}_h \in \mathbf{V}_h \\ (\nabla \cdot \mathbf{q}_h, w_h)_K + (c u_h, w_h)_K + \langle \tau (u_h - \hat{u}_h), w_h \rangle_{\partial K} &= 0 \quad \forall w_h \in W_h. \end{aligned}$$

If $\hat{u}_h|_{\partial K} \in \mathbb{R}_k(\partial K)$ is represented with a vector $\mathbf{u}_{\partial K} \in \mathbb{R}^{4d_2}$, then the matrix representation of this local solution is

$$\begin{bmatrix} \mathbf{q}_K \\ \mathbf{u}_K \end{bmatrix} = -(\mathbb{A}_1^K)^{-1} \mathbb{A}_2^K \mathbf{u}_{\partial K} \in \mathbb{R}^{3d_3 + d_3}$$

If we consider the $4d_3 \times N_{\text{elt}}$ matrix with columns

$$\mathbb{A}_f^K := \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{f}^K \end{bmatrix},$$

then

$$\begin{bmatrix} \mathbf{q}_K \\ \mathbf{u}_K \end{bmatrix} = (\mathbb{A}_1^K)^{-1} \mathbb{A}_f^K$$

are the coefficients of the solution of

$$\begin{aligned} (\kappa^{-1} \mathbf{q}_h, \mathbf{r}_h)_K - (u_h, \nabla \cdot \mathbf{r}_h)_K &= 0 \quad \forall \mathbf{r}_h \in \mathbf{V}_h \\ (\nabla \cdot \mathbf{q}_h, w_h)_K + (c u_h, w_h)_K + \langle \tau u_h, w_h \rangle_{\partial K} &= (f, w_h)_K \quad \forall w_h \in W_h. \end{aligned}$$

7.3 Flux operators

Consider now the $4d_2 \times 4d_3 \times N_{\text{elt}}$ array with slices

$$\mathbb{A}_3^K := \begin{bmatrix} n_x \text{DP}^K & n_y \text{DP}^K & n_z \text{DP}^K & \tau \text{DP}^K \end{bmatrix},$$

the $4d_2 \times 4d_2 \times N_{\text{elt}}$ array with slices

$$\mathbb{C}^K := \mathbb{A}_3^K (\mathbb{A}_1^K)^{-1} \mathbb{A}_2^K + \tau \text{DD}^K$$

and the $4d_2 \times N_{\text{elt}}$ matrix with columns

$$\mathbb{C}_f^K := \mathbb{A}_3^K (\mathbb{A}_1^K)^{-1} \mathbb{A}_f^K.$$

The meaning of these matrices can be made clear by looking at boundary fluxes.

Flux due to \hat{u}_h . Given $(\mathbf{q}_h, u_h, \hat{u}_h) \in \mathbf{V}_h \times W_h \times M_h$, the HDG is based on the construction of the function

$$\mathbf{q}_h \cdot \boldsymbol{\nu} + \tau(u_h - \hat{u}_h) : \partial K \rightarrow \mathbb{R}.$$

Instead of this quantity, we pay attention to how it creates a linear form

$$\mathcal{R}_k(\partial K) \ni \hat{v}_h \longmapsto -\langle \mathbf{q}_h \cdot \boldsymbol{\nu} + \tau(u_h - \hat{u}_h), \hat{v}_h \rangle_{\partial K} = -\langle \mathbf{q}_h \cdot \boldsymbol{\nu} + \tau u_h, \hat{v}_h \rangle_{\partial K} + \langle \tau \hat{u}_h, \hat{v}_h \rangle_{\partial K},$$

whose matrix representation is

$$-\mathbb{A}_3^K \begin{bmatrix} \mathbf{q}_K \\ \mathbf{u}_K \end{bmatrix} + (\tau \text{DD})^K \mathbf{u}_{\partial K} = \mathbb{A}_3^K (\mathbb{A}_1^K)^{-1} \mathbb{A}_2^K \mathbf{u}_{\partial K} + (\tau \text{DD})^K \mathbf{u}_{\partial K} = \mathbb{C}^K \mathbf{u}_{\partial K}$$

Flux due to sources. If we take (\mathbf{q}_h, u_h) by solving the local equations due to sources and consider the linear form

$$\mathcal{R}_k(\partial K) \ni \hat{v}_h \longmapsto \langle \mathbf{q}_h \cdot \boldsymbol{\nu} + \tau u_h, \hat{v}_h \rangle_{\partial K},$$

(\hat{u}_h does not appear here), then the matrix representation of this is

$$\mathbb{A}_3^K \begin{bmatrix} \mathbf{q}_K \\ \mathbf{u}_K \end{bmatrix} = \mathbb{A}_3^K (\mathbb{A}_1^K)^{-1} \mathbb{A}_f^K = \mathbb{C}_f^K.$$

If we solve the local problems ($\hat{u}_h \in M_h$ and f are given)

$$\begin{aligned} (\kappa^{-1} \mathbf{q}_h, \mathbf{r}_h)_K - (u_h, \nabla \cdot \mathbf{r}_h)_K + \langle \hat{u}_h, \mathbf{r}_h \cdot \boldsymbol{\nu} \rangle_{\partial K} &= 0 & \forall \mathbf{r}_h \in \mathbf{V}_h \\ (\nabla \cdot \mathbf{q}_h, w_h)_K + (c u_h, w_h)_K + \langle \tau(u_h - \hat{u}_h), w_h \rangle_{\partial K} &= (f, w_h)_K & \forall w_h \in W_h, \end{aligned}$$

then the functional

$$\mathcal{R}_k(\partial K) \ni \hat{v}_h \longmapsto \langle \mathbf{q}_h \cdot \boldsymbol{\nu} + \tau u_h, \hat{v}_h \rangle_{\partial K},$$

has the matrix representation

$$\mathbb{C}^K \mathbf{u}_{\partial K} - \mathbb{C}_f^K,$$

where $\mathbf{u}_{\partial K}$ is the vector of degrees of freedom of $\hat{u}_h|_{\partial K}$.

Implementation notes. Note that the Matlab expression A_3/A_1*A_2 corresponds to $A_3A_1^{-1}A_2$ (no inversion of A_1 is required in the process). *The loop over elements can be parallelized in a very simple way.*

```
function [C,Cf,A1,A2,Af]=localsolvers3d(km,c,f,tau,T,k,formulas)

%[C,Cf,A1,A2,Af]=localsolvers3d(km,c,f,tau,T,k,{for1,for2,for3})
%
%Input:
%      km, c, f: vectorized functions of three variables
%      tau: penalization parameter for HDG (Nelts x 4)
%      T: expanded tetrahedrization
%      k: polynomial degree
%      for1: quadrature formula 3d (for mass matrix)
%      for2: quadrature formula 3d (for convection matrices)
%      for3: quadrature formula 2d
%
%Output:
%      C:      4*d2 x 4*d2 x Nelts
%      Cf:     4*d2 x Nelts
%      A1:     4*d3 x 4*d3 x Nelts
%      A2:     4*d3 x 4*d2 x Nelts
%      Af:     4*d3 x Nelts
%
%Last modified: Nov 29, 2012

Nelts=size(T.elements,1);
d2=nchoosek(k+2,2);
d3=nchoosek(k+3,3);

f=testElem(f,T,k,formulas{1});
Af=zeros(4*d3,Nelts);
Af(3*d3+1:4*d3,:)=f;

Mass=MassMatrix(T,{km,c},k,formulas{1});
Mk=Mass{1};Mc=Mass{2};
[Cx,Cy,Cz]=ConvMatrix(T,k,formulas{2});
[tauPP,tauDP,nxDP,nyDP,nzDP,tauDD]=matricesFace(T,tau,k,formulas{3});

A1=zeros(4*d3,4*d3,Nelts);
A2=zeros(4*d3,4*d2,Nelts);
C=zeros(4*d2,4*d2,Nelts);
Cf=zeros(4*d2,Nelts);

O=zeros(d3,d3,Nelts);
A1=[Mk      ,O      ,O      ,-permute(Cx,[2 1 3]);...
    O      ,Mk      ,O      ,-permute(Cy,[2 1 3]);...
    O      ,O      ,Mk      ,-permute(Cz,[2 1 3]);...
    Cx      ,Cy      ,Cz      ,Mc+tauPP];
A2=[permute(nxDP,[2 1 3]);...
    permute(nyDP,[2 1 3]);...
    permute(nzDP,[2 1 3]);...
    -permute(tauDP,[2 1 3])];

parfor i=1:Nelts
    C(:, :, i)=[nxDP(:, :, i) nyDP(:, :, i) nzDP(:, :, i) tauDP(:, :, i)]/A1(:, :, i)*A2(:, :, i)...
               +tauDD(:, :, i);
    Cf(:, i)=[nxDP(:, :, i) nyDP(:, :, i) nzDP(:, :, i) tauDP(:, :, i)]/A1(:, :, i)*Af(:, i);
end
return
```

8 Boundary conditions

8.1 Dirichlet boundary conditions

The discretization of the Dirichlet boundary condition is given by projecting the Dirichlet data u_D on the space

$$M_h^{\text{dir}} := \prod_{e \in \mathcal{E}_h^{\text{dir}}} \mathcal{P}_k(e) \quad \dim M_h^{\text{dir}} = d_2 N_{\text{dir}}.$$

We have to find values

$$u_j^e \quad j = 1, \dots, d_2, \quad e \in \mathcal{E}_h^{\text{dir}} \quad \widehat{u}_h|_e = \sum_j u_j^e D_j^e$$

such that

$$\sum_j \left(\int_e D_i^e D_j^e \right) u_j^e = \int_e D_i^e \widehat{u}_h = \int_e D_i^e u_D, \quad i = 1, \dots, d_2, \quad e \in \mathcal{E}_h^{\text{dir}}.$$

Using a quadrature rule, this is equivalent (up to quadrature error) to solving the system

$$|e| \sum_{j=1}^{d_2} \left(\sum_r \varpi_r \widehat{D}_i(\widehat{\mathbf{q}}_r) \widehat{D}_j(\widehat{\mathbf{q}}_r) \right) u_j^e = |e| \sum_r \varpi_r \widehat{D}_i(\widehat{\mathbf{q}}_r) u_D(\widehat{\mathbf{q}}_r), \quad i = 1, \dots, d_2, \quad e \in \mathcal{E}_h^{\text{dir}}.$$

If we compute three $N_{\text{qd}} \times N_{\text{dir}}$ matrices $\mathbf{X}^{\text{dir}}, \mathbf{Y}^{\text{dir}}, \mathbf{Z}^{\text{dir}}$ and the basic $N_{\text{qd}} \times d_2$ matrices on the reference element

$$\mathbf{D}_{ri} := \widehat{D}_i(\widehat{\mathbf{q}}_r)$$

then the entire computation is reduced to

$$((\boldsymbol{\varpi} \odot \mathbf{D})^\top \mathbf{D})^{-1} (\boldsymbol{\varpi} \odot \mathbf{D})^\top u_D(\mathbf{X}^{\text{dir}}, \mathbf{Y}^{\text{dir}}, \mathbf{Z}^{\text{dir}}).$$

8.2 Neumann boundary conditions

We will be imposing boundary conditions in the form

$$\kappa \nabla u \cdot \boldsymbol{\nu} = \mathbf{u}_N \cdot \boldsymbol{\nu} \quad \text{or equivalently} \quad -\mathbf{q} \cdot \boldsymbol{\nu} = \mathbf{u}_N \cdot \boldsymbol{\nu}.$$

This is done in this non-standard form in order to simplify the inclusion of complicated solutions. The aim of this part of the code is the computation of the $d_2 \times N_{\text{neu}}$ matrix

$$\int_e (\mathbf{u}_N \cdot \boldsymbol{\nu}) D_i^e \quad i = 1, \dots, d_2, \quad e \in \mathcal{E}_h^{\text{neu}}.$$

Using a quadrature rule we can approximate

$$\int_e (\mathbf{u}_N \cdot \boldsymbol{\nu}) D_i^e \approx \sum_r \mathbf{u}_N(\mathbf{q}_r^e) \cdot \mathbf{n}^e \varpi_r \widehat{D}_i(\widehat{\mathbf{q}}_r).$$

If $\mathbf{u}_N = (u_x, u_y, u_z)$ and \mathbf{n}_\star are column vectors with the \star components of the normal vectors of each of the N_{neu} Neumann faces, then, we just need to compute

$$\sum_{\star \in \{x, y, z\}} \mathbf{n}_\star^\top \odot ((\boldsymbol{\varpi} \odot \mathbf{D})^\top u_\star(\mathbf{X}^{\text{neu}}, \mathbf{Y}^{\text{neu}}, \mathbf{Z}^{\text{neu}})),$$

where $\mathbf{X}^{\text{neu}}, \mathbf{Y}^{\text{neu}}, \mathbf{Z}^{\text{neu}}$ are $N_{\text{qd2}} \times N_{\text{neu}}$ matrices with the coordinates of all quadrature points on the Neumann faces.

```

function [uhd,qhn]=BC3d(uD,gx,gy,gz,T,k,formula)

%[uhd,qhn]=BC3d(uD,gx,gy,gz,T,k,formula)
%
% Input:
%       uD: Dirichlet data; vectorized function of three variables
%       gx,gy,gz: Neumann data (corresponds to kappa*grad(u))
%               vectorized functions of three variables
%       T: Full tetrahedrization
%       k: polynomial degree
%       formula: quadrature formula in 2d (N x 4 matrix)
%
% Output:
%       uhd: d2 x Ndir,    Ndir, number of Dirichlet faces
%       qhn: d2 x Nneu,    Nneu, number of Neumann faces
%
% Last modified: March 21, 2013

x=T.coordinates(:,1);
y=T.coordinates(:,2);
z=T.coordinates(:,3);

%Dirichlet
xx=formula(:, [1 2 3])*x(T.dirichlet'); % Nnodes x Ndir
yy=formula(:, [1 2 3])*y(T.dirichlet'); % Nnodes x Ndir
zz=formula(:, [1 2 3])*z(T.dirichlet'); % Nnodes x Ndir
D=dubiner2d(2*formula(:,2)-1,2*formula(:,3)-1,k); % Nnodes x d2
wD=bsxfun(@times,formula(:,4),D); % Nnodes x d2
uhd=(wD'*D)\uD(xx,yy,zz);

%Neumann
x12=x(T.neumann(:,2))-x(T.neumann(:,1)); %x2-x1
y12=y(T.neumann(:,2))-y(T.neumann(:,1)); %y2-y1
z12=z(T.neumann(:,2))-z(T.neumann(:,1)); %z2-z1
x13=x(T.neumann(:,3))-x(T.neumann(:,1)); %x3-x1
y13=y(T.neumann(:,3))-y(T.neumann(:,1)); %y3-y1
z13=z(T.neumann(:,3))-z(T.neumann(:,1)); %z3-z1

Neu.normals=0.5*[y12.*z13-z12.*y13,...
                z12.*x13-x12.*z13,...
                x12.*y13-x13.*y12]; % Nneu x 3, ||n^e||=|e|

xn=formula(:, [1 2 3])*x(T.neumann'); % Nnodes x Nneu
yn=formula(:, [1 2 3])*y(T.neumann'); % Nnodes x Nneu
zn=formula(:, [1 2 3])*z(T.neumann'); % Nnodes x Nneu

qhn=bsxfun(@times,Neu.normals(:,1)',wD'*gx(xn,yn,zn))+...
      bsxfun(@times,Neu.normals(:,2)',wD'*gy(xn,yn,zn))+...
      bsxfun(@times,Neu.normals(:,3)',wD'*gz(xn,yn,zn)); %d2 x Nneu
return

```

9 HDG

For the correct definition of the HDG method, we need to consider the space

$$M_h^{\text{free}} := \{\hat{v}_h \in M_h : \hat{v}_h|_{\Gamma_D} = 0\} = \prod_{e \in \mathcal{E}_h^{\text{free}}} \mathcal{P}_k(e), \quad \text{where} \quad \text{free} := \{1, \dots, N_{\text{fc}}\} \setminus \text{dir}.$$

The HDG method looks for $\hat{u}_h \in M_h$ such that

$$\langle \hat{u}_h, \hat{v}_h \rangle_{\Gamma_D} = \langle u_D, \hat{v}_h \rangle_{\Gamma_D} \quad \forall \hat{v}_h \in M_h^{\text{dir}}$$

(this is the discrete Dirichlet BC), and

$$-\sum_{K \in \mathcal{T}_h} \langle \mathbf{q}_h \cdot \boldsymbol{\nu} + \tau(u_h - \hat{u}_h), \hat{v}_h \rangle_{\partial K} = \langle \mathbf{u}_N \cdot \boldsymbol{\nu}, \hat{v}_h \rangle_{\Gamma_N} \quad \forall \hat{v}_h \in M_h^{\text{free}},$$

where $(\mathbf{q}_h, u_h) \in \mathbf{V}_h \times W_h$ is the solution of the local problems:

$$\begin{aligned} (\kappa^{-1} \mathbf{q}_h, \mathbf{r}_h)_K - (u_h, \nabla \cdot \mathbf{r}_h)_K + \langle \hat{u}_h, \mathbf{r}_h \cdot \boldsymbol{\nu} \rangle_{\partial K} &= 0 \quad \forall \mathbf{r}_h \in \mathcal{P}_k(K)^3, \\ (\nabla \cdot \mathbf{q}_h, w_h)_K + (c u_h, w_h)_K + \langle \tau(u_h - \hat{u}_h), w_h \rangle_{\partial K} &= (f, w_h)_K \quad \forall w_h \in \mathcal{P}_k(K) \end{aligned}$$

for all $K \in \mathcal{T}_h$. The global equation can be decomposed in two groups: for interior faces $e = K \cap \tilde{K}$, we can write

$$-\langle \mathbf{q}_K \cdot \boldsymbol{\nu}_K + \tau_K(u_K - \hat{u}_e), \hat{v}_e \rangle_e - \langle \mathbf{q}_{\tilde{K}} \cdot \boldsymbol{\nu}_{\tilde{K}} + \tau_{\tilde{K}}(u_{\tilde{K}} - \hat{u}_e), \hat{v}_e \rangle_e = 0 \quad \forall \hat{v}_e \in \mathcal{P}_k(e),$$

(this is equality of discrete fluxes across inter-element faces), and for Neumann faces $e \in \mathcal{E}_h^{\text{neu}}$, $e \subset \partial K$, we have a discretized version of the Neumann BC

$$-\langle \mathbf{q}_K \cdot \boldsymbol{\nu}_K + \tau_K(u_K - \hat{u}_e), \hat{v}_e \rangle_e = \langle \mathbf{u}_N \cdot \boldsymbol{\nu}_e, \hat{v}_e \rangle_e \quad \forall \hat{v}_e \in \mathcal{P}_k(e).$$

Since we are testing with the space M_h^{free} , all integrals on Dirichlet faces are ignored after assembly, while values of \hat{u}_h on Dirichlet faces are substituted from the Dirichlet BC.

9.1 Assembly process

The local solvers produce a $4d_2 \times 4d_2 \times N_{\text{elt}}$ array \mathbb{C} . We now use the **sparse** Matlab builder to assembly the global matrix. The degrees of freedom associated to face $e \in \{1, \dots, N_{\text{fc}}\}$ are

$$\text{list}(e) = (e-1)d_2 + \{1, \dots, d_2\}.$$

The degrees of freedom associated to the faces of K are thus

$$\text{dof}(K) := \{\text{list}(e_1^K), \text{list}(e_2^K), \text{list}(e_3^K), \text{list}(e_4^K)\}.$$

We then create two new $4d_2 \times 4d_2 \times N_{\text{elt}}$ arrays

$$\text{Row}_{ij}^K = \text{dof}(K)_i \quad \text{Col}_{ij}^K = \text{dof}(K)_j.$$

Note that the element (i, j) of \mathbb{C}^K has to be assembled at the location $(\text{Row}_{ij}^K, \text{Col}_{ij}^K) = (\text{dof}(K)_i, \text{dof}(K)_j)$. The assembly of the **source term**, given in the matrix \mathbb{C}_f , can be carried out using the **accumarray** command. The element $(\mathbb{C}_f^K)_i$ has to be added to the location $\text{dof}(K)_i$.

9.2 The global system

1. The assembly process of the \mathbb{C}^K matrices produces an $N_{\text{fc}} \times N_{\text{fc}}$ matrix. Similarly, the accumulation of the \mathbb{C}_f^K vectors produces a vector with N_{fc} components. On the Neumann components of this vector, we have to add a vector, with the tests of $\mathbf{u}_N \cdot \boldsymbol{\nu}$ on Neumann faces.

2. The value of the unknown on Dirichlet faces is substituted from the data given by the Dirichlet BC and the corresponding part of the system is send to the right hand side. The rows associated to the Dirichlet faces are eliminated from the system (this is the same process that is applied to Dirichlet BC in the Finite Element Method). The system is solved on the free degrees of freedom.

3. The solution of the resulting system is $\hat{u}_h \in M_h$. Reconstruction of the other variables (\mathbf{q}_h, u_h) is done by solving local problems. In matrix form, we have to solve on each $K \in \mathcal{T}_h$ the system

$$\mathbb{A}_1^K \begin{bmatrix} \mathbf{q}_K \\ \mathbf{u}_K \end{bmatrix} = \mathbb{A}_f^K - \mathbb{A}_2^K \mathbf{u}_{\partial K}.$$

Implementation notes. The necessary quadrature formulas are brought in a cell array:

`{formula1,formula2,formula3,formula4}`

as follows:

- **formula1** is used for mass matrices; it is assumed to be of degree $3k$ at least; it is also used for all error computations
- **formula2** is used for convection matrices (with constant coefficients); it is assumed to be of degree $2k$ at least
- **formula3** is a 2-dimensional formula used for integrals on faces; it is assumed to be of degree $2k$ at least
- **formula4** is a higher order 2-dimensional formula used for errors

For input we bring in:

- the coefficients and source term: κ^{-1}, c, f ;
- the penalization parameter function τ in the form of a $N_{\text{elt}} \times 4$ matrix; the choice of a matrix with all unit entries works fine
- the functions for the boundary conditions u_D and (g_x, g_y, g_z) (recall that we impose a boundary condition $-\mathbf{q} \cdot \boldsymbol{\nu} = \kappa \nabla u \cdot \boldsymbol{\nu} = \mathbf{g} \cdot \boldsymbol{\nu}$)
- an optional parameter:
 - if the parameter is not present or its value is zero, then the problem is solved and the solution is exported in five variables corresponding to matrix forms for u_h , the components of \mathbf{q}_h and \hat{u}_h
 - if the parameter is not zero, then the system is not solved, but the elements of the system (the matrix, the right hand side and the lists of degrees of freedom (not faces) that are free and Dirichlet) are exported, as well as the local solvers \mathbb{A}_1 , \mathbb{A}_2 and \mathbb{A}_f , that are needed to reconstruct the solution.

```
function [Uh,Qxh,Qyh,Qzh,Uhat,system,solvers]=HDG3d(km,c,f,tau,T,k,formulas,uD,gx,gy,gz,varargin)

%[Uh,Qxh,Qyh,Qzh,Uhat]=HDG3d(km,c,f,tau,T,k,formulas,uD,gx,gy,gz)
%[Uh,Qxh,Qyh,Qzh,Uhat]=HDG3d(km,c,f,tau,T,k,formulas,uD,gx,gy,gz,0)
%[-,-,-,-,-,system,solvers]=HDG3d(km,c,f,tau,T,k,formulas,uD,gx,gy,gz,1)
%
%Input:
%      km   : vectorized function (kappa^{-1}; kappa=diffusion parameter)
%      c    : vectorized function (reaction parameter)
%      f    : vectorized function (source term)
%      tau  : penalization parameter for HDG (Nelts x 4)
%      T    : expanded tetrahedrization
%      k    : polynomial degree
%      formulas: {for1,for2,for3}
%              (quadrature formulas as used by localsolvers3d)
%      uD   : Dirichlet data; vectorized function
%      gx,gy,gz : Neumann data (corresponds to kappa*grad(u)); vectorized fns
%
%Output:
%      Uh    : d3 x Nelts,    matrix with uh
%      Qxh   : d3 x Nelts,    matrix with qxh
%      Qyh   : d3 x Nelts,    matrix with qyh
```

```

%      Qzh      : d3 x Nelts,    matrix with qzh
%      Uhat     : d2 x Nelts    matrix with uhat
%      system   : {HDGmatrix,HDGrhs,list of free d.o.f.,list of dir d.o.f.}
%      solvers   : {A1,A2,Af}    local solvers
%
%Last modified: April 11, 2013

if nargin==12
    export=varargin{1};
else
    export=0;
end

d2=nchoosek(k+2,2);
d3=nchoosek(k+3,3);
block3=@(x) (1+(x-1)*d3):(x*d3);
Nelts =size(T.elements,1);
Nfaces=size(T.faces,1);
Ndir  =size(T.dirichlet,1);
Nneu  =size(T.neumann,1);

%Matrices for assembly process

face=T.facebyele';    % 4 x Nelts
face=(face(:)-1)*d2;  % First degree of freedom of each face by element
face=bsxfun(@plus,face,1:d2);    %4*Nelts x d2 (d.o.f. for each face)
face=reshape(face',4*d2,Nelts);  %d.o.f. for the 4 faces of each element

[J,I]=meshgrid(1:4*d2);
R=face(I(:),:); R=reshape(R,4*d2,4*d2,Nelts);
C=face(J(:),:); C=reshape(C,4*d2,4*d2,Nelts);
    % R_ij^K d.o.f. for local (i,j) d.o.f. in element K ; R_ij^K=C_ji^K
RowsRHS=reshape(face,4*d2*Nelts,1);

dirfaces=(T.dirfaces(:)-1)*d2;
dirfaces=bsxfun(@plus,dirfaces,1:d2);
dirfaces=reshape(dirfaces',d2*Ndir,1);

free=((1:Nfaces)-1)*d2;
free=bsxfun(@plus,free,1:d2);
free=reshape(free',d2*Nfaces,1);
free(dirfaces)=[];

neufaces=(T.neufaces(:)-1)*d2;
neufaces=bsxfun(@plus,neufaces,1:d2);
neufaces=reshape(neufaces',d2*Nneu,1);

%Local solvers and global system

[M1,Cf,A1,A2,Af]=localsolvers3d(km,c,f,tau,T,k,formulas);
M=sparse(R(:),C(:),M1(:));
phif=accumarray(RowsRHS,Cf(:));

[uhatD,qhatN]=BC3d(uD,gx,gy,gz,T,k,formulas{3});

%Dirichlet BC
Uhatv=zeros(d2*Nfaces,1);
Uhatv(dirfaces)=uhatD;    %uhat stored as a vector: d2*Nfaces

%RHS
rhs=zeros(d2*Nfaces,1);
rhs(free)=phif(free);
qhatN=reshape(qhatN,d2*Nneu,1);    % qhatN stored as a vector: d2*Nneu
rhs(neufaces)=rhs(neufaces)+qhatN;
rhs=rhs-M(:,dirfaces)*Uhatv(dirfaces);

```

```

if export
    system={M, rhs, free, dirfaces};
    solvers={A1, A2, Af};
    Uh=[];
    Qxh=[];
    Qyh=[];
    Qzh=[];
    Uhat=[];
    return
else
    system=[];
    solvers=[];
end

Uhatv(free)=M(free, free)\rhs(free);
Uhat=reshape(Uhatv, d2, Nfaces);

%Uh Qxh Qyh Qzh

faces=T.facebyele'; faces=faces(:);
uhhataux=reshape(Uhat(:, faces), [4*d2, Nelts]);
sol=zeros(4*d3, Nelts);
parfor K=1:Nelts
    sol(:, K)=A1(:, :, K)\(Af(:, K)-A2(:, :, K)*uhhataux(:, K));
end

Qxh=sol(block3(1), :);
Qyh=sol(block3(2), :);
Qzh=sol(block3(3), :);
Uh =sol(block3(4), :);
return

```

10 Local projections

10.1 L^2 projection on elements

Given $u : \Omega \rightarrow \mathbb{R}$ we look for u_h (given by coefficients u_j^K) such that

$$\sum_j \left(\int_K P_i^K P_j^K \right) u_j^K = \int_K P_i^K u_h = \int_K P_i^K u \quad i = 1, \dots, d_3, \quad K \in \mathcal{T}_h.$$

Using a quadrature rule, we can compute

$$\int_K P_i^K P_j^K = |K| \sum_q \hat{\omega}_q \hat{P}_i(\hat{\mathbf{p}}_q) \hat{P}_j(\hat{\mathbf{p}}_q),$$

and approximate

$$\int_K P_i^K u \approx |K| \sum_q \hat{\omega}_q \hat{P}_i(\hat{\mathbf{p}}_q) u(\mathbf{p}_q^K)$$

so that, with the $N_{\text{qd}} \times N_{\text{elt}}$ matrices of coordinates of all quadrature points on all elements, we can just compute

$$((\hat{\omega} \odot \mathbf{P})^\top \mathbf{P})^{-1} (\hat{\omega} \odot \mathbf{P})^\top u(\mathbf{X}, \mathbf{Y}, \mathbf{Z}).$$

```

function [fh,error]=L2proj3d(f,T,k,formula1,formula2)

%[fh,error]=L2proj3d(f,T,k,formula1,formula2)
%
%Input:

```

```

%           f: vectorized function of three variables
%           T: full tetrahedrization
%           k: polynomial degree
%   formula1: quadrature formula in 3d
%   formula2: quadrature formula in 3d to compute errors
%
%Output:
%           fh: L2 projection of f ; disc P_k function (d3 x Nelts)
%           error: L^2 error
%
%Last modified: April 2, 2013

P =dubiner3d(2*formula2(:,2)-1,2*formula2(:,3)-1,2*formula2(:,4)-1,k);
wP=bsxfun(@times,formula2(:,5),P);
x=T.coordinates(:,1); x=formula2(:,1:4)*x(T.elements');
y=T.coordinates(:,2); y=formula2(:,1:4)*y(T.elements');
z=T.coordinates(:,3); z=formula2(:,1:4)*z(T.elements');

fh=(wP'*P)\wP'*f(x,y,z);
error=errorElem(T,f,fh,k,formula1);
return

```

10.2 L^2 projection on the skeleton

Given $u : \Omega \rightarrow \mathbb{R}$, we look for $\hat{u}_h \in M_h$ (given by coefficients u_j^e) such that

$$\sum_j \left(\int_e D_i^e D_j^e \right) u_j^e = \int_e D_i^e \hat{u}_h = \int_e D_i^e u \quad i = 1, \dots, d_2, \quad e \in \mathcal{E}_h.$$

Using a quadrature formula we compute

$$\int_e D_i^e D_j^e = |e| \sum_r \varpi_r \hat{D}_i(\hat{\mathbf{q}}_r) \hat{D}_j(\hat{\mathbf{q}}_r)$$

and approximate

$$\int_e D_i^e u \approx |e| \sum_r \varpi_r \hat{D}_i(\hat{\mathbf{q}}_r) u(\hat{\mathbf{q}}_r^e).$$

Therefore, we just have to compute

$$((\boldsymbol{\varpi} \odot \mathbf{D})^\top \mathbf{D})^{-1} (\boldsymbol{\varpi} \odot \mathbf{D})^\top u(\mathbf{X}, \mathbf{Y}, \mathbf{Z}),$$

after computing the matrices with the coordinates of all quadrature points in all elements.

```

function [fh,error]=L2projskeleton3d(f,T,k,formula1,formula2)

%[fh,error]=L2projskeleton3d(f,T,k,formula1,formula2)
%
%Input:
%           f: vectorized function of three variables
%           T: expanded tetrahedrization
%           k: polynomial degree
%   formula1: quadrature formula in 2d
%   formula2: quadrature formula in 2d to compute errors
%
%Output:
%           fh: L2 projection on the skeleton (d2 x Nfaces)
%           error: h-weighted error
%
%Last modified: April 2, 2013

```

```

D =dubiner2d(2*formula1(:,2)-1,2*formula1(:,3)-1,k);    %Nnodes x d2
wD=bsxfun(@times,formula1(:,4),D);
x=T.coordinates(:,1); x=formula1(:,1:3)*x(T.faces(:,1:3)');
y=T.coordinates(:,2); y=formula1(:,1:3)*y(T.faces(:,1:3)');
z=T.coordinates(:,3); z=formula1(:,1:3)*z(T.faces(:,1:3)');

fh=( (wD'*D)\wD')*f(x,y,z);

error=errorFaces(T,f,fh,k,formula2);
return

```

10.3 The HDG projection

Given a pair (\mathbf{q}, u) (a vector field and a function), the HDG projection is the discrete pair $(\mathbf{q}_h, u_h) \in \mathbf{V}_h \times W_h$ such that

$$\begin{aligned}
(\mathbf{q}_h, \mathbf{r}_h)_K &= (\mathbf{q}, \mathbf{r}_h)_K & \forall \mathbf{r}_h \in \mathcal{P}_{k-1}(K)^3, \\
(u_h, w_h)_K &= (u, w_h)_K & \forall w_h \in \mathcal{P}_{k-1}(K), \\
\langle \mathbf{q}_h \cdot \boldsymbol{\nu} + \tau u_h, \hat{v}_h \rangle_{\partial K} &= \langle \mathbf{q} \cdot \boldsymbol{\nu} + \tau u, \hat{v}_h \rangle_{\partial K} & \forall \hat{v}_h \in \mathcal{R}_k(\partial K),
\end{aligned}$$

for all $K \in \mathcal{T}_h$. This problem can be decomposed in a sequence of N_{elt} linear systems of order $4d_3$. We first compute a constant mass matrix \mathbf{M}^K (in the usual $d_3 \times d_3 \times N_{\text{elt}}$ format) and drop the last d_2 rows, to get a $(d_3 - d_2) \times d_3 \times N_{\text{elt}}$ array with slices $\tilde{\mathbf{M}}^K$. (Note that $\dim \mathcal{P}_k(K) - \dim \mathcal{P}_{k-1}(K) = d_2$. In the case $k = 0$, $\tilde{\mathbf{M}}$ is an empty matrix.)

The matrix to that appears in the left hand side of each of the local projectors is the $(4(d_3 - d_2) + 4d_2) \times 4d_3$ block matrix

$$\begin{bmatrix}
\tilde{\mathbf{M}}^K & \mathbf{O} & \mathbf{O} & \mathbf{O} \\
\mathbf{O} & \tilde{\mathbf{M}}^K & \mathbf{O} & \mathbf{O} \\
\mathbf{O} & \mathbf{O} & \tilde{\mathbf{M}}^K & \mathbf{O} \\
\mathbf{O} & \mathbf{O} & \mathbf{O} & \tilde{\mathbf{M}}^K \\
n_x \mathbf{DP}^K & n_y \mathbf{DP}^K & n_z \mathbf{DP}^K & \tau \mathbf{DP}^K
\end{bmatrix}$$

The first four blocks of the right hand side (for the element K) correspond to the tests

$$\int_K q_x P_i^K, \quad \int_K q_y P_i^K, \quad \int_K q_z P_i^K, \quad \int_K u P_i^K, \quad i = 1, \dots, d_3 - d_2.$$

```

function [Pqx,Pqy,Pqz,Pu]=projectHDG3d(T,coeffs,k,tau,formulas)

%[Pqx,Pqy,Pqz,Pu]=projectHDG3d(T,coeffs,k,tau,formulas)
%
%Input:
%      T: Tetrahedrization
%      coeffs: each cell is a vectorized function of three variables
%      k: degree of polynomial
%      formulas: quadrature matrix for mass matrix and convection matrix
%
%Output:
%      Pqx: \Pi qx,
%      Pqy: \Pi qy,
%      Pqz: \Pi qz,
%      Pu: \Pi u,

%Last modified: April 9, 2013

d2=nchoosek(k+2,2);

```

```

d3=nchoosek(k+3,3); %Nbasis
if k>0
    d4=nchoosek(k+2,3); %dim P_{k-1}(K)
else
    d4=0;
end
block3=@(x) (1+(x-1)*d3):(x*d3);
a=@(x,y,z) 1+0.*x;

Mass=MassMatrix(T,{a},k,formulas{1});

Mass=Mass{1};
rows=1+d4:d3;
Mass(rows,:,:)=[];

[tauPP,tauDP,nxDP,nyDP,nzDP]=matricesFace(T,tau,k,formulas{3});
Nelts=size(T.elements,1);
O=zeros(d4,d3,Nelts);
M=[Mass O O O ;
    O Mass O O ;
    O O Mass O ;
    O O O Mass;
    nxDP nyDP nzDP tauDP];

if k>0
    Ints=testElem(coeffs,T,k-1,formulas{2});
    qxP=Ints{1};
    qyP=Ints{2};
    qzP=Ints{3};
    uP=Ints{4};
else
    qxP=zeros(0,Nelts);
    qyP=zeros(0,Nelts);
    qzP=zeros(0,Nelts);
    uP=zeros(0,Nelts);
end

Ints=testFaces(coeffs,T,k,formulas{3});
qxD=Ints{1};
qyD=Ints{2};
qzD=Ints{3};
uD=Ints{4};

nx=T.normals(:, [1 4 7 10]);
ny=T.normals(:, [2 5 8 11]);
nz=T.normals(:, [3 6 9 12]);
nx=nx./T.area(T.facebyele);
ny=ny./T.area(T.facebyele);
nz=nz./T.area(T.facebyele);

QxD=zeros(d2,4,Nelts);
QyD=QxD;
QzD=QxD;
UD =QxD;

Pqx=zeros(d3,Nelts);
Pqy=Pqx;
Pqz=Pqx;
Pu =Pqx;

parfor i=1:Nelts
    QxD(:, :, i)=bsxfun(@times, QxD(:, T.facebyele(i, :)), nx(i, :));
    QyD(:, :, i)=bsxfun(@times, QyD(:, T.facebyele(i, :)), ny(i, :));
    QzD(:, :, i)=bsxfun(@times, QzD(:, T.facebyele(i, :)), nz(i, :));
    UD(:, :, i)=bsxfun(@times, ud(:, T.facebyele(i, :)), tau(:, i)');
    qxv=QxD(:, :, i);

```

```

    qyv=QyD(:, :, i);
    qzv=QzD(:, :, i);
    uv=UD(:, :, i);

    rhs=[qxP(:, i);
        qyP(:, i);
        qzP(:, i);
        uP(:, i);
        qxv(:)+qyv(:)+qzv(:)+uv(:)];
    vect=M(:, :, i)\rhs;

    Pqx(:, i)=vect(block3(1));
    Pqy(:, i)=vect(block3(2));
    Pqz(:, i)=vect(block3(3));
    Pu(:, i)=vect(block3(4));
end
return

```

11 Preprocessing of the triangulation

The first part of the code is quite technical and could possibly be optimized. We start by constructing `T.faces`, the list of all faces. The way this is constructed, the list contains:

- first all the interior faces; for each of the faces, the nodes are given in increasing order;
- then the Dirichlet faces, preserving the ordering that was given as input
- then the Neumann faces, preserving the ordering that was given as input.

The HDG code does not use these particularities of the construction of the list of faces. We next construct the list `T.facebyele` by backward referencing from the original lists. The last delicate part of the code is the construction of `T.perm`. Other than that, everything is relatively straightforward.

```

function T=HDGgrid3d(T,positive)
%
% T=HDGgrid3d(T,p)
%
% Input:
%   T : Basic tetrahedral data structure
%   p : 1 if boundary faces are positively oriented
%       -1 otherwise
% Output:
%   T : Expanded tetrahedral data structure
%
% Last modified: May 2, 2012
%

if positive~=1
    T.dirichlet(:, [2 3])=T.dirichlet(:, [3 2]);
    T.neumann(:, [2 3])=T.neumann(:, [3 2]);
end

% Construction of a list of all faces

shape=[1 3 2;1 2 4;1 4 3;2 3 4];
nelts=size(T.elements,1);
faces=zeros(4*nelts,3);
for k=1:nelts
    nodes=T.elements(k, :); %1x4
    faces(4*(k-1)+(1:4), :)=nodes(shape); % 1x3
end
copyoffaces=faces; % 4 nelts x 3 (in local positive orientation)

```

```

faces=sort(faces,2);
[allfaces,i,j]=unique(faces,'rows');

% Lists of interior and boundary faces with references

bdfaces=sort([T.dirichlet;T.neumann],2);
[intfaces,i]=setdiff(allfaces,bdfaces,'rows');
[bdfaces,ii,jj]=intersect(allfaces,bdfaces,'rows');

nintfaces=size(intfaces,1);
ndirfaces=size(T.dirichlet,1);
nneufaces=size(T.neumann,1);
nbdfaces =size(bdfaces,1);
nfaces   =nintfaces+nbdfaces;

T.faces=[intfaces zeros(nintfaces,1);...
         T.dirichlet ones(ndirfaces,1);...
         T.neumann 2*ones(nneufaces,1)];
T.dirfaces=(nintfaces+1):(nintfaces+ndirfaces);
T.neufaces=(nintfaces+ndirfaces+1):(nintfaces+ndirfaces+nneufaces);

% Backward referencing to construct T.facebyele

u=zeros(nfaces,1);
v=nintfaces+1:nintfaces+nbdfaces;
u(i)=1:nintfaces;
u(ii)=v(jj);
j=u(j); % pointer from T.faces to the copyoffaces
faces=T.faces(j,1:3); % 4 nelts x 3, with global numbering of nodes
j=reshape(j,[4 nelts]);
T.facebyele=j';

% Matrix with orientations

A=T.facebyele';
faces=T.faces(A(:,1:3));
t=sum(faces==copyoffaces,2)==ones(4*nelts,1);
t=1-2*t;t=reshape(t,[4,nelts]);
T.orientation=t';

% Matrix with permutation order

eq = @(u,v) sum(u==v,2)==3; % checks what rows are equal
rot=[1 2 3;... % permutations
     1 3 2;...
     3 1 2;...
     3 2 1;...
     2 3 1;...
     2 1 3];
pattern=[1 2 3;... % (s,t,0)
         1 2 4;... % (s,0,t)
         1 3 4;... % (0,s,t)
         4 2 3]; % (s,t,1-s-t)
orient=zeros(nelts,4);

for f=1:4 % counter over faces
    faceGlobal=T.faces(T.facebyele(:,f),1:3);
    faceLocal =T.elements(:,pattern(f,:));
    for j=1:6
        orient(:,f)=orient(:,f)+j*eq(faceGlobal,faceLocal(:,rot(j,:)));
    end
end
T.perm=orient;

% Volumes and areas

```

```

T.volume=(1/6)*...
((T.coordinates(T.elements(:,2),1)-T.coordinates(T.elements(:,1),1)).*...
(T.coordinates(T.elements(:,3),2)-T.coordinates(T.elements(:,1),2)).*...
(T.coordinates(T.elements(:,4),3)-T.coordinates(T.elements(:,1),3))-...
(T.coordinates(T.elements(:,2),1)-T.coordinates(T.elements(:,1),1)).*...
(T.coordinates(T.elements(:,3),3)-T.coordinates(T.elements(:,1),3)).*...
(T.coordinates(T.elements(:,4),2)-T.coordinates(T.elements(:,1),2))-...
(T.coordinates(T.elements(:,2),2)-T.coordinates(T.elements(:,1),2)).*...
(T.coordinates(T.elements(:,3),1)-T.coordinates(T.elements(:,1),1)).*...
(T.coordinates(T.elements(:,4),3)-T.coordinates(T.elements(:,1),3))+...
(T.coordinates(T.elements(:,2),2)-T.coordinates(T.elements(:,1),2)).*...
(T.coordinates(T.elements(:,3),3)-T.coordinates(T.elements(:,1),3)).*...
(T.coordinates(T.elements(:,4),1)-T.coordinates(T.elements(:,1),1))+...
(T.coordinates(T.elements(:,2),3)-T.coordinates(T.elements(:,1),3)).*...
(T.coordinates(T.elements(:,3),1)-T.coordinates(T.elements(:,1),1)).*...
(T.coordinates(T.elements(:,4),2)-T.coordinates(T.elements(:,1),2))-...
(T.coordinates(T.elements(:,2),3)-T.coordinates(T.elements(:,1),3)).*...
(T.coordinates(T.elements(:,3),2)-T.coordinates(T.elements(:,1),2)).*...
(T.coordinates(T.elements(:,4),1)-T.coordinates(T.elements(:,1),1)));

T.area=(1/2)*sqrt(...
((T.coordinates(T.faces(:,2),2)-T.coordinates(T.faces(:,1),2)).*...
(T.coordinates(T.faces(:,3),3)-T.coordinates(T.faces(:,1),3))-...
(T.coordinates(T.faces(:,2),3)-T.coordinates(T.faces(:,1),3)).*...
(T.coordinates(T.faces(:,3),2)-T.coordinates(T.faces(:,1),2))).^2+...
((T.coordinates(T.faces(:,2),1)-T.coordinates(T.faces(:,1),1)).*...
(T.coordinates(T.faces(:,3),3)-T.coordinates(T.faces(:,1),3))-...
(T.coordinates(T.faces(:,2),3)-T.coordinates(T.faces(:,1),3)).*...
(T.coordinates(T.faces(:,3),1)-T.coordinates(T.faces(:,1),1))).^2+...
((T.coordinates(T.faces(:,2),1)-T.coordinates(T.faces(:,1),1)).*...
(T.coordinates(T.faces(:,3),2)-T.coordinates(T.faces(:,1),2))-...
(T.coordinates(T.faces(:,2),2)-T.coordinates(T.faces(:,1),2)).*...
(T.coordinates(T.faces(:,3),1)-T.coordinates(T.faces(:,1),1))).^2);

%Normals to the faces
for f=1:4
    oneface=T.faces(T.facebyele(:,f),1:3);
    x=T.coordinates(oneface(:,1));
    y=T.coordinates(oneface(:,2));
    z=T.coordinates(oneface(:,3));
    %
    x12=x(nelts+1:2*nelts)-x(1:nelts); %x_2-x_1
    x13=x(2*nelts+1:end)-x(1:nelts); %x_3-x_1
    y12=y(nelts+1:2*nelts)-y(1:nelts); %y_2-y_1
    y13=y(2*nelts+1:end)-y(1:nelts); %y_3-y_1
    z12=z(nelts+1:2*nelts)-z(1:nelts); %z_2-z_1
    z13=z(2*nelts+1:end)-z(1:nelts); %z_3-z_1
    %
    normals=(1/2)*[y12.*z13-y13.*z12,...
        z12.*x13-z13.*x12,...
        x12.*y13-x13.*y12];
    normals=bsxfun(@times,normals,T.orientation(:,f)); % Give the normals correctly orientated
    %
    T.normals(:,(f-1)*3+(1:3))=normals;
end
return

```

12 Matrices for convection-diffusion

12.1 Variable convection

In order to compute convection matrices with a variable coefficient

$$\int_K c P_i^K \partial_\star P_j^K \quad i, j, = 1, \dots, d_3, \quad K \in \mathcal{T}_h, \quad \star \in \{x, y, z\},$$

we proceed like in Section 5.5, but looping on quadrature nodes. Using notation of Section 5.5, we can write

$$\begin{aligned} \int_K c P_i^K P_{j,\star}^K &= \sum_{\# = 1}^3 a_{\star\#}^K \int_{\hat{K}} (c \circ F_K) \hat{P}_i \hat{P}_{j,\#} \\ &\approx \frac{1}{6} \sum_{\# = 1}^3 \sum_q a_{\star\#}^q c(\mathbf{p}_q^K) (\hat{C}_q^\#)_{ij}, \quad (\hat{C}_q^\#)_{ij} := \hat{\omega}_q \hat{P}_i(\hat{\mathbf{p}}_q) \hat{P}_{j,\#}(\hat{\mathbf{p}}_q). \end{aligned}$$

This means that we need to compute $3N_{\text{qd}}$ ($d_3 \times d_3$) matrices on the reference element (the matrices $\hat{C}_q^\#$) and use them for $3N_{\text{qd}}$ Kronecker products in order to compute a particular value of \star . In total, there will be $9N_{\text{qd}}$ Kronecker products.

As for the vector involved in the Kronecker products, they are the columns of $\mathbf{a}_{\star\#} \odot c(\mathbf{X}, \mathbf{Y}, \mathbf{Z})$, where $\mathbf{a}_{\star\#}$ are the *column* vectors with the geometric coefficients of the change of variables and $\mathbf{X}, \mathbf{Y}, \mathbf{Z}$ are the $N_{\text{qd}} \times N_{\text{elt}}$ matrices with the coordinates of the quadrature points.

Implementation notes. Thinking of convection-diffusion problems, the code provides convection matrices with different parameter functions for each of the variables, that is

$$\int_K v_x P_i^K \partial_x P_j^K \quad \int_K v_y P_i^K \partial_y P_j^K \quad \int_K v_z P_i^K \partial_z P_j^K.$$

The variables $\mathbf{a}, \mathbf{b}, \mathbf{c}, \dots$ are used to tag the nine components of $\det \mathbf{B}_K \mathbf{B}_K^{-\top}$ read by rows (see Section 5.5) as $N_{\text{elt}} \times 1$ vectors. The capitalized forms $\mathbf{A}, \mathbf{B}, \dots$ correspond to $N_{\text{elt}} \times N_{\text{qd}}$ arrays with the values of the variable coefficient at all quadrature points. For instance $\mathbf{a}, \mathbf{b}, \mathbf{c}$ corresponding to elements of the first row (and thus to a C^x matrix), they have to be multiplied by the value of v_x at quadrature points.

```
function [convx,convy,convz]=VariableConv(T,vx,vy,vz,k,formula)

%[convx,convy,convz]=VariableConv(T,vx,vy,vz,k,formula)
%
%Input:
%   T: expanded tetrahedrization
%   vx,vy,vz: vectorized functions of three variables
%   k: polynomial degree
%   formula: quadrature formula in 3d (N x 5 matrix)
%
%Output:
%   convx: d3 x d3 x Nelts ( \int_K vx P_i^K \partial_x P_j^K )
%   convy: d3 x d3 x Nelts ( \int_K vy P_i^K \partial_y P_j^K )
%   convz: d3 x d3 x Nelts ( \int_K vz P_i^K \partial_z P_j^K )
%
%Last modified: May 31, 2012

Nelts=size(T.elements,1);
Nnodes=size(formula,1);
d3=nchoosek(k+3,3);
```

```

x=T.coordinates(:,1);x=x(T.elements)*formula(:,1:4)'; %Nelts x Nnodes
y=T.coordinates(:,2);y=y(T.elements)*formula(:,1:4)';
z=T.coordinates(:,3);z=z(T.elements)*formula(:,1:4)';

convx=zeros(d3,Nelts*d3);
convy=zeros(d3,Nelts*d3);
convz=zeros(d3,Nelts*d3);

xhat=formula(:,2);
yhat=formula(:,3);
zhat=formula(:,4);

[p,px,py,pz]=dubiner3d(2*xhat-1,2*yhat-1,2*zhat-1,k); % Nnodes x d3
px=2*px;
py=2*py;
pz=2*pz;

x12=T.coordinates(T.elements(:,2),1)-T.coordinates(T.elements(:,1),1); %x2-x1
x13=T.coordinates(T.elements(:,3),1)-T.coordinates(T.elements(:,1),1); %x3-x1
x14=T.coordinates(T.elements(:,4),1)-T.coordinates(T.elements(:,1),1); %x4-x1
y12=T.coordinates(T.elements(:,2),2)-T.coordinates(T.elements(:,1),2); %y2-y1
y13=T.coordinates(T.elements(:,3),2)-T.coordinates(T.elements(:,1),2); %y3-y1
y14=T.coordinates(T.elements(:,4),2)-T.coordinates(T.elements(:,1),2); %y4-y1
z12=T.coordinates(T.elements(:,2),3)-T.coordinates(T.elements(:,1),3); %z2-z1
z13=T.coordinates(T.elements(:,3),3)-T.coordinates(T.elements(:,1),3); %z3-z1
z14=T.coordinates(T.elements(:,4),3)-T.coordinates(T.elements(:,1),3); %z4-z1

a=y13.*z14-y14.*z13;
b=y14.*z12-y12.*z14;
c=y12.*z13-y13.*z12;
d=x14.*z13-x13.*z14;
e=x12.*z14-x14.*z12;
f=x13.*z12-x12.*z13;
g=x13.*y14-x14.*y13;
h=x14.*y12-x12.*y14;
i=x12.*y13-x13.*y12;

A=bsxfun(@times,a,vx(x,y,z));
B=bsxfun(@times,b,vx(x,y,z));
C=bsxfun(@times,c,vx(x,y,z));
D=bsxfun(@times,d,vy(x,y,z));
E=bsxfun(@times,e,vy(x,y,z));
F=bsxfun(@times,f,vy(x,y,z));
G=bsxfun(@times,g,vz(x,y,z));
H=bsxfun(@times,h,vz(x,y,z));
I=bsxfun(@times,i,vz(x,y,z));

for i=1:Nnodes
    convx=convx+kron(A(:,i)',1/6*formula(i,5)*p(i,:)'*px(i,:))+...
        kron(B(:,i)',1/6*formula(i,5)*p(i,:)'*py(i,:))+...
        kron(C(:,i)',1/6*formula(i,5)*p(i,:)'*pz(i,:));
    convy=convy+kron(D(:,i)',1/6*formula(i,5)*p(i,:)'*px(i,:))+...
        kron(E(:,i)',1/6*formula(i,5)*p(i,:)'*py(i,:))+...
        kron(F(:,i)',1/6*formula(i,5)*p(i,:)'*pz(i,:));
    convz=convz+kron(G(:,i)',1/6*formula(i,5)*p(i,:)'*px(i,:))+...
        kron(H(:,i)',1/6*formula(i,5)*p(i,:)'*py(i,:))+...
        kron(I(:,i)',1/6*formula(i,5)*p(i,:)'*pz(i,:));
end
convx=reshape(convx,[d3,d3,Nelts]);
convy=reshape(convy,[d3,d3,Nelts]);
convz=reshape(convz,[d3,d3,Nelts]);
return

```

12.2 Face matrices related to convection

The first collection of matrices is a generalization of what we called the Type (c) matrices in Section 6.4. The goal is the approximate computation of

$$\frac{\xi_\ell^K}{|e_\ell^K|} \int_{e_\ell^K} \alpha D_i^{e_\ell^K} P_j^K \quad \begin{array}{l} i = 1, \dots, d_2 \\ j = 1, \dots, d_3 \end{array} \quad \ell \in \{1, 2, 3, 4\}, \quad K \in \mathcal{T}_h,$$

where $\xi \in \mathcal{P}_0(\partial\mathcal{T}_h)$, and α is a function of three variables. The result will be presented as a $(4d_2) \times d_3 \times N_{\text{elt}}$ array, by stacking the blocks for $\ell \in \{1, 2, 3, 4\}$ on top of each other ($\ell = 1$ on top). Most of what we next explain is an easy generalization of what appears in Section 6.4.

We first compute the evaluation matrices (see Section 3.3 for the quadrature nodes on the boundary of the reference tetrahedron)

$$\begin{aligned} P_{ri}^\ell &:= \widehat{P}_i(\widehat{\mathbf{q}}_r^\ell) & i = 1, \dots, d_3, \quad r = 1, \dots, N_{\text{qd2}}, \quad \ell \in \{1, 2, 3, 4\}, \\ D_{ri}^\mu &:= \widehat{D}_i(F_\mu(\widehat{\mathbf{q}}_r)) & i = 1, \dots, d_2, \quad r = 1, \dots, N_{\text{qd2}}, \quad \mu \in \{1, 2, 3, 4, 5, 6\}. \end{aligned}$$

We next consider the piecewise constant functions $\xi_\mu \in \mathcal{P}_0(\partial\mathcal{T}_h)$ given by

$$\xi_{\ell,\mu}^K = \xi_\ell^K \mathbf{1}_{\text{perm}(K,\ell)=\mu} = \begin{cases} \xi_\ell^K & \text{if } \text{perm}(K,\ell) = \mu, \\ 0, & \text{otherwise.} \end{cases}$$

If $X^\mathcal{T}, Y^\mathcal{T}, Z^\mathcal{T}$ are the $4 \times N_{\text{elt}}$ matrices with the coordinates of the vertices of the elements and Ω_ℓ is the $N_{\text{qd2}} \times 4$ matrix with the barycentric coordinates of the points $\{\widehat{\mathbf{q}}_r^\ell\}$, we then construct the $N_{\text{qd2}} \times N_{\text{elt}}$ matrices

$$A_\ell := \alpha(\Omega_\ell X^\mathcal{T}, \Omega_\ell Y^\mathcal{T}, \Omega_\ell Z^\mathcal{T}) \quad \ell \in \{1, 2, 3, 4\},$$

containing the values of α in all quadrature points. The computation is then

$$\sum_{\mu=1}^6 (\mathbf{a}_{\ell,r}^\top \bullet \xi_{\mu,r}^\top) \otimes \left((D^\mu)^\top (\varpi \odot P^\ell) \right), \quad \mathbf{a}_{\ell,r}^\top := \text{Row}(A_\ell, r), \quad \xi_{\mu,r}^\top := \text{Row}(\xi_\mu, r),$$

where the symbol \bullet has been used to denote the element-by-element multiplication of two arrays.

Implementation notes. Instead of doing the computation for a single function α paired with a single piecewise constant function ξ , the code runs for a cell array of functions α paired with a cell array of piecewise constant functions ξ .

```
function mat=matricesVariableFaceA(T,a1,pw,k,formula)

% {m1,m2,...}=matricesFaceVariable(T,{a1,a2,...},{pw1,pw2...},k,form)
%
% Input:
%   T           : full tetrahedrization
%   a1,a2,...   : vectorized function of three variables
%   pw1,pw2,... : piecewise constant function on skeleton 4 x Nfaces
%   k           : polynomial degree
%   form        : 2-dimensional quadrature rule
% Output:
%   m1,m2,...   : 4d2 x d3 x Nelts
%
% Last modified: April 5, 2013

% Evaluations of Dubiner3d functions on all faces

Nelts=size(T.elements,1);
Nnodes=size(formula,1);
```

```

T.perm=T.perm'; % 4 x Nelts

d2=nchoosek(k+2,2);
d3=nchoosek(k+3,3);

s=formula(:,2);
t=formula(:,3);
O=zeros(size(s));
points3d=[s,t,O;...
          s,O,t;...
          O,s,t;...
          s,t,1-s-t];

P =dubiner3d(2*points3d(:,1)-1,2*points3d(:,2)-1,2*points3d(:,3)-1,k);
wP=bsxfun(@times,[formula(:,4);...
                  formula(:,4);...
                  formula(:,4);...
                  formula(:,4)],P);

% Evaluations of alpha on all faces

x=T.coordinates(:,1);
y=T.coordinates(:,2);
z=T.coordinates(:,3);
points3d=[1-sum(points3d,2) points3d]; % barycentric coordinates
x=points3d*x(T.elements');
y=points3d*y(T.elements');
z=points3d*z(T.elements');

% Evaluations of Dubiner2d polynomials on six different configurations

points2d=[s,t;...
          t,s;...
          1-s-t,s;...
          s,1-s-t;...
          t,1-s-t;...
          1-s-t,t];
D=dubiner2d(2*points2d(:,1)-1,2*points2d(:,2)-1,k); % 6*Nnodes x d2

% Construction of the matrix

for c=1:length(al)
    alpha=al{c};
    alpha=alpha(x,y,z); % 4Nnodes X Nelts
    pwct =pw{c};
    matrix=zeros(4*d2,d3*Nelts);
    for l=1:4
        rows=1+(l-1)*d2:(l*d2);
        for mu=1:6
            pwctmu=pwct(l,:).*(T.perm(l,:)==mu);
            for r=1:Nnodes
                rowP=(l-1)*Nnodes+r;
                rowD=(mu-1)*Nnodes+r;
                matrix(rows,:)=matrix(rows,...
                    +kron(pwctmu.*alpha(rowP,:),D(rowD,:))*wP(rowP,:));
            end
        end
    end
    mat{c}=reshape(matrix,[4*d2,d3,Nelts]);
end

```

The following step concerns the generalization of the Type (b) matrices of Section 6.4 to variable coefficients. We show how to approximate

$$\frac{\xi_\ell^K}{|e_\ell^K|} \int_{e_\ell^K} \alpha D_i^{e_\ell^K} D_j^{e_\ell^K} \quad i, j = 1, \dots, d_2 \quad \ell \in \{1, 2, 3, 4\}, \quad K \in \mathcal{T}_h,$$

where $\xi \in \mathcal{P}_0(\partial\mathcal{T}_h)$, and α is a function of three variables. The result will be given as a block diagonal $(4d_2) \times (4d_2) \times N_{\text{elt}}$ array, by daigonally stacking the blocks for different values of ℓ . We start by computing the values of α on all quadrature nodes: the $N_{\text{qd2}} \times N_{\text{fc}}$ matrix

$$A := \alpha(\Xi X^\mathcal{E}, \Xi Z^\mathcal{E}, \Xi Y^\mathcal{E})$$

(where $X^\mathcal{E}, Y^\mathcal{E}, Z^\mathcal{E}$ are $3 \times N_{\text{fc}}$ with the coordinates of all vertices of all faces and Ξ is the $N_{\text{qd2}} \times 3$ matrix with the barycentric coordinates of the quadrature points $\hat{\mathbf{q}}_r$), is organized by global number of faces. We can then construct (by choosing columns in a proper way) for $N_{\text{qd2}} \times N_{\text{elt}}$ matrices A_ℓ such that

$$A_{\ell,r}^K = A_{r,e_\ell^K} \quad r = 1, \dots, N_{\text{qd2}}, \quad K \in \mathcal{T}_h, \quad \ell \in \{1, 2, 3, 4\}.$$

(The information needed for this is contained in `T.facebyele(:,1)`.) Finally we compute

$$\sum_r (\mathbf{a}_{\ell,r}^\top \bullet \xi_\ell^\top) \otimes (\varpi_r \mathbf{d}_r \mathbf{d}_r^\top), \quad \mathbf{a}_{\ell,r}^\top := \text{Row}(A_\ell, r), \quad \xi_\ell^\top := \text{Row}(\xi, \ell), \quad \mathbf{d}_r^\top := \text{Row}(\mathbf{D}, r).$$

Implementation notes. Instead of doing the computation for a single function α paired with a single piecewise constant function ξ , the code runs for a cell array of functions α paired with a cell array of piecewise constant functions ξ .

```
function mat=matricesVariableFaceB(T,al,pw,k,formula)

% {m1,m2,...}=matricesFaceVariable(T,{a1,a2,...},{pw1,pw2,...},k,form)
%
% Input:
%   T           : full tetrahedrization
%   al,a2,...   : vectorized function of three variables
%   pw1,pw2,... : piecewise constant function on skeleton 4 x Nfaces
%   k           : polynomial degree
%   form        : 2-dimensional quadrature rule
% Output:
%   m1,m2,...   : 4d2 x 4d2 x Nelts
%
% Last modified: April 2, 2013

% Parameters

Nelts=size(T.elements,1);
Nnodes=size(formula,1);
d2=nchoosek(k+2,2);
O=zeros(d2,d2,Nelts);

% Evaluations of alpha and Dubiner 2d on all faces

x=T.coordinates(:,1);x=formula(:,1:3)*x(T.faces(:,1:3)');
y=T.coordinates(:,2);y=formula(:,1:3)*y(T.faces(:,1:3)');
z=T.coordinates(:,3);z=formula(:,1:3)*z(T.faces(:,1:3)');
D=dubiner2d(2*formula(:,2)-1,2*formula(:,3)-1,k);

% Construction of the matrix

for c=1:length(al);
    alpha=al{c};
    alpha=alpha(x,y,z);           % Nnodes X Nfaces
    pwct=pw{c};
    for l=1:4
        dgm{1}=zeros(d2,d2*Nelts);
        for r=1:Nnodes
            dgm{1}=dgm{1}+...
                kron(pwct(1,:).*alpha(r,T.facebyele(:,1)),...
                    formula(r,4)*D(r,:)'*D(r,:));
        end
    end
end
```

```

end
dgm{1}=reshape(dgm{1},[d2,d2,Nelts]);
end
mat{c}=[dgm{1} 0 0 0 ; ...
0 dgm{2} 0 0 ; ...
0 0 dgm{3} 0 ; ...
0 0 0 dgm{4}];
end
return

```

13 Postprocessing

13.1 Local stiffness matrices

The goal of this section is the computation of the matrices

$$\int_K \nabla P_i^K \cdot \nabla P_j^K \quad i, j = 1, \dots, d_3, \quad K \in \mathcal{T}_h.$$

For differentiation indices, let us identify the sets $(x, y, z) \equiv (1, 2, 3)$. We consider the canonical basis of the space of matrices

$$E_{\star\#} = \mathbf{e}_\star \mathbf{e}_\#^\top, \quad \star, \# \in \{x, y, z\}.$$

For instance

$$E_{xy} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

We need to compute six 3×3 geometric matrices:

$$G_{\star\#}^K = |\det B_K|^2 B_K^{-1} E_{\star\#} B_K^{-\top}, \quad \star, \# \in \{x, y, z\}, \quad K \in \mathcal{T}_h.$$

We will give explicit formulas for these matrices below. Note that

$$(G_{\star\#}^K)^\top = |\det B_K|^2 (B_K^{-1} E_{\star\#} B_K^{-\top})^\top = |\det B_K|^2 B_K^{-1} E_{\star\#}^\top B_K^{-\top} = G_{\#\star}^K,$$

which is the reason why only six of them are needed/computed. Besides, the matrices $G_{\star\star}^T$ are symmetric. Once we have computed these matrices, we can obtain

$$\begin{aligned}
(S_{\star\#}^K)_{ij} &= \int_K \partial_\star P_i^K \partial_\# P_j^K = \int_K (\nabla P_i^K) \cdot (E_{\star\#} \nabla P_j^K) \\
&= |\det B_K| \int_{\hat{K}} (B_K^{-\top} \nabla \hat{P}_i) \cdot (E_{\star\#} B_K^{-\top} \nabla \hat{P}_j) \\
&= |\det B_K|^{-1} \int_{\hat{K}} (\nabla \hat{P}_i) \cdot (G_{\star\#}^K \nabla \hat{P}_j) \\
&= |\det B_K|^{-1} \sum_{\alpha, \beta \in \{x, y, z\}} (G_{\star\#}^K)_{\alpha, \beta} \int_{\hat{K}} (\nabla \hat{P}_i) \cdot (E_{\alpha, \beta} \nabla \hat{P}_j) \\
&= |\det B_K|^{-1} \sum_{\alpha, \beta \in \{x, y, z\}} (G_{\star\#}^K)_{\alpha, \beta} \int_{\hat{K}} \partial_\alpha \hat{P}_i \partial_\beta \hat{P}_j.
\end{aligned}$$

The elements of the matrices $G_{\star\#}^K$ are polynomial expressions of the elements of B_K .

$$G_{xx}^K = \begin{bmatrix} (y_{13} z_{14} - z_{13} y_{14})^2 & (y_{13} z_{14} - z_{13} y_{14})(-y_{12} z_{14} + z_{12} y_{14}) & (y_{13} z_{14} - z_{13} y_{14})(y_{12} z_{13} - z_{12} y_{13}) \\ (y_{13} z_{14} - z_{13} y_{14})(-y_{12} z_{14} + z_{12} y_{14}) & (-y_{12} z_{14} + z_{12} y_{14})^2 & (-y_{12} z_{14} + z_{12} y_{14})(y_{12} z_{13} - z_{12} y_{13}) \\ (y_{13} z_{14} - z_{13} y_{14})(y_{12} z_{13} - z_{12} y_{13}) & (-y_{12} z_{14} + z_{12} y_{14})(y_{12} z_{13} - z_{12} y_{13}) & (y_{12} z_{13} - z_{12} y_{13})^2 \end{bmatrix}$$

$$G_{xy}^K = \begin{bmatrix} (y_{13} z_{14} - z_{13} y_{14})(-x_{13} z_{14} + z_{13} x_{14}) & (y_{13} z_{14} - z_{13} y_{14})(x_{12} z_{14} - z_{12} x_{14}) & (y_{13} z_{14} - z_{13} y_{14})(-x_{12} z_{13} + z_{12} x_{13}) \\ (-x_{13} z_{14} + z_{13} x_{14})(-y_{12} z_{14} + z_{12} y_{14}) & (-y_{12} z_{14} + z_{12} y_{14})(x_{12} z_{14} - z_{12} x_{14}) & (-y_{12} z_{14} + z_{12} y_{14})(-x_{12} z_{13} + z_{12} x_{13}) \\ (-x_{13} z_{14} + z_{13} x_{14})(y_{12} z_{13} - z_{12} y_{13}) & (x_{12} z_{14} - z_{12} x_{14})(y_{12} z_{13} - z_{12} y_{13}) & (y_{12} z_{13} - z_{12} y_{13})(-x_{12} z_{13} + z_{12} x_{13}) \end{bmatrix}$$

$$G_{xz}^K = \begin{bmatrix} (y_{13} z_{14} - z_{13} y_{14})(x_{13} y_{14} - y_{13} x_{14}) & (y_{13} z_{14} - z_{13} y_{14})(-x_{12} y_{14} + y_{12} x_{14}) & (y_{13} z_{14} - z_{13} y_{14})(x_{12} y_{13} - y_{12} x_{13}) \\ (x_{13} y_{14} - y_{13} x_{14})(-y_{12} z_{14} + z_{12} y_{14}) & (-y_{12} z_{14} + z_{12} y_{14})(-x_{12} y_{14} + y_{12} x_{14}) & (-y_{12} z_{14} + z_{12} y_{14})(x_{12} y_{13} - y_{12} x_{13}) \\ (x_{13} y_{14} - y_{13} x_{14})(y_{12} z_{13} - z_{12} y_{13}) & (-x_{12} y_{14} + y_{12} x_{14})(y_{12} z_{13} - z_{12} y_{13}) & (y_{12} z_{13} - z_{12} y_{13})(x_{12} y_{13} - y_{12} x_{13}) \end{bmatrix}$$

$$G_{yy}^K = \begin{bmatrix} (-x_{13} z_{14} + z_{13} x_{14})^2 & (-x_{13} z_{14} + z_{13} x_{14})(x_{12} z_{14} - z_{12} x_{14}) & (-x_{13} z_{14} + z_{13} x_{14})(-x_{12} z_{13} + z_{12} x_{13}) \\ (-x_{13} z_{14} + z_{13} x_{14})(x_{12} z_{14} - z_{12} x_{14}) & (x_{12} z_{14} - z_{12} x_{14})^2 & (x_{12} z_{14} - z_{12} x_{14})(-x_{12} z_{13} + z_{12} x_{13}) \\ (-x_{13} z_{14} + z_{13} x_{14})(-x_{12} z_{13} + z_{12} x_{13}) & (x_{12} z_{14} - z_{12} x_{14})(-x_{12} z_{13} + z_{12} x_{13}) & (-x_{12} z_{13} + z_{12} x_{13})^2 \end{bmatrix}$$

$$G_{yz}^K = \begin{bmatrix} (-x_{13} z_{14} + z_{13} x_{14})(x_{13} y_{14} - y_{13} x_{14}) & (-x_{13} z_{14} + z_{13} x_{14})(-x_{12} y_{14} + y_{12} x_{14}) & (-x_{13} z_{14} + z_{13} x_{14})(x_{12} y_{13} - y_{12} x_{13}) \\ (x_{13} y_{14} - y_{13} x_{14})(x_{12} z_{14} - z_{12} x_{14}) & (x_{12} z_{14} - z_{12} x_{14})(-x_{12} y_{14} + y_{12} x_{14}) & (x_{12} z_{14} - z_{12} x_{14})(x_{12} y_{13} - y_{12} x_{13}) \\ (x_{13} y_{14} - y_{13} x_{14})(-x_{12} z_{13} + z_{12} x_{13}) & (-x_{12} y_{14} + y_{12} x_{14})(-x_{12} z_{13} + z_{12} x_{13}) & (-x_{12} z_{13} + z_{12} x_{13})(x_{12} y_{13} - y_{12} x_{13}) \end{bmatrix}$$

$$G_{zz}^K = \begin{bmatrix} (x_{13} y_{14} - y_{13} x_{14})^2 & (x_{13} y_{14} - y_{13} x_{14})(-x_{12} y_{14} + y_{12} x_{14}) & (x_{13} y_{14} - y_{13} x_{14})(x_{12} y_{13} - y_{12} x_{13}) \\ (x_{13} y_{14} - y_{13} x_{14})(-x_{12} y_{14} + y_{12} x_{14}) & (-x_{12} y_{14} + y_{12} x_{14})^2 & (-x_{12} y_{14} + y_{12} x_{14})(x_{12} y_{13} - y_{12} x_{13}) \\ (x_{13} y_{14} - y_{13} x_{14})(x_{12} y_{13} - y_{12} x_{13}) & (-x_{12} y_{14} + y_{12} x_{14})(x_{12} y_{13} - y_{12} x_{13}) & (x_{12} y_{13} - y_{12} x_{13})^2 \end{bmatrix}$$

The stiffness matrix is the sum

$$S_{xx}^K + S_{yy}^K + S_{zz}^K.$$

```
function S=Stiffness(T,k,formula)

% S=stiffness(T,k,formula)
%
% Input:
%   T      : tetrahedrization
%   k      : polynomial degree
%   formula : quadrature formula
% Output:
%   S      : d3 x d3 x Nelts stiffness matrix
% Last modified: March 27, 2013

% Computations in the reference element

xhat=formula(:,2);
yhat=formula(:,3);
zhat=formula(:,4);

[~,px,py,pz]=dubiner3d(2*xhat-1,2*yhat-1,2*zhat-1,k);
px=2*px; wpx=bsxfun(@times,formula(:,5),px);
py=2*py; wpy=bsxfun(@times,formula(:,5),py);
pz=2*pz; wpz=bsxfun(@times,formula(:,5),pz);

Kxx=(1/6)*px'*wpx;
Kxy=(1/6)*px'*wpy;
Kxz=(1/6)*px'*wpz;
Kyy=(1/6)*py'*wpy;
Kyz=(1/6)*py'*wpz;
Kzz=(1/6)*pz'*wpz;

% Geometric constructions

x12=T.coordinates(T.elements(:,2),1)-T.coordinates(T.elements(:,1),1);
y12=T.coordinates(T.elements(:,2),2)-T.coordinates(T.elements(:,1),2);
z12=T.coordinates(T.elements(:,2),3)-T.coordinates(T.elements(:,1),3);
x13=T.coordinates(T.elements(:,3),1)-T.coordinates(T.elements(:,1),1);
y13=T.coordinates(T.elements(:,3),2)-T.coordinates(T.elements(:,1),2);
z13=T.coordinates(T.elements(:,3),3)-T.coordinates(T.elements(:,1),3);
x14=T.coordinates(T.elements(:,4),1)-T.coordinates(T.elements(:,1),1);
```

```

y14=T.coordinates(T.elements(:,4),2)-T.coordinates(T.elements(:,1),2);
z14=T.coordinates(T.elements(:,4),3)-T.coordinates(T.elements(:,1),3);
x12=x12'; x13=x13'; x14=x14';
y12=y12'; y13=y13'; y14=y14';
z12=z12'; z13=z13'; z14=z14'; % row vectors with differences of coords

idetB=1./(x12.*y13.*z14-x12.*y14.*z13-y12.*x13.*z14...
+y12.*x14.*z13+z12.*x13.*y14-z12.*x14.*y13);

dxdx=kron(idetB.*(y13.*z14-z13.*y14).^2,Kxx)...
+kron(idetB.*(y13.*z14-z13.*y14).*(-y12.*z14+z12.*y14),Kxy+Kxy')...
+kron(idetB.*(y13.*z14-z13.*y14).*(y12.*z13-z12.*y13),Kxz+Kxz')...
+kron(idetB.*(-y12.*z14+z12.*y14).^2,Kyy)...
+kron(idetB.*(-y12.*z14+z12.*y14).*(y12.*z13-z12.*y13),Kyz+Kyz')...
+kron(idetB.*(y12.*z13-z12.*y13).^2,Kzz);
dydy=kron(idetB.*(-x13.*z14+z13.*x14).^2,Kxx)...
+kron(idetB.*(-x13.*z14+z13.*x14).*(x12.*z14-z12.*x14),Kxy+Kxy')...
+kron(idetB.*(-x13.*z14+z13.*x14).*(-x12.*z13+z12.*x13),Kxz+Kxz')...
+kron(idetB.*(x12.*z14-z12.*x14).^2,Kyy)...
+kron(idetB.*(x12.*z14-z12.*x14).*(-x12.*z13+z12.*x13),Kyz+Kyz')...
+kron(idetB.*(-x12.*z13+z12.*x13).^2,Kzz);
dzdz=kron(idetB.*(x13.*y14-y13.*x14).^2,Kxx)...
+kron(idetB.*(x13.*y14-y13.*x14).*(-x12.*y14+y12.*x14),Kxy+Kxy')...
+kron(idetB.*(x13.*y14-y13.*x14).*(x12.*y13-y12.*x13),Kxz+Kxz')...
+kron(idetB.*(-x12.*y14+y12.*x14).^2,Kyy)...
+kron(idetB.*(-x12.*y14+y12.*x14).*(x12.*y13-y12.*x13),Kyz+Kyz')...
+kron(idetB.*(x12.*y13-y12.*x13).^2,Kzz);

S=dxdx+dydy+dzdz;
d3=nchoosek(k+3,3);
Nelts=size(T.elements,1);
S=reshape(S,[d3 d3 Nelts]);

return

% These matrices are not needed

dxdy=kron(idetB.*(y13.*z14-z13.*y14).*(-x13.*z14+z13.*x14),Kxx)...
+kron(idetB.*(y13.*z14-z13.*y14).*(x12.*z14-z12.*x14),Kxy)...
+kron(idetB.*(y13.*z14-z13.*y14).*(-x12.*z13+z12.*x13),Kxz)...
+kron(idetB.*(-x13.*z14+z13.*x14).*(-y12.*z14+z12.*y14),Kxy')...
+kron(idetB.*(-y12.*z14+z12.*y14).*(x12.*z14-z12.*x14),Kyy)...
+kron(idetB.*(-y12.*z14+z12.*y14).*(-x12.*z13+z12.*x13),Kyz)...
+kron(idetB.*(-x13.*z14+z13.*x14).*(y12.*z13-z12.*y13),Kxz')...
+kron(idetB.*(x12.*z14-z12.*x14).*(y12.*z13-z12.*y13),Kyz')...
+kron(idetB.*(y12.*z13-z12.*y13).*(-x12.*z13+z12.*x13),Kzz);
dxdz=kron(idetB.*(y13.*z14-z13.*y14).*(x13.*y14-y13.*x14),Kxx)...
+kron(idetB.*(y13.*z14-z13.*y14).*(-x12.*y14+y12.*x14),Kxy)...
+kron(idetB.*(y13.*z14-z13.*y14).*(x12.*y13-y12.*x13),Kxz)...
+kron(idetB.*(x13.*y14-y13.*x14).*(-y12.*z14+z12.*y14),Kxy')...
+kron(idetB.*(-y12.*z14+z12.*y14).*(-x12.*y14+y12.*x14),Kyy)...
+kron(idetB.*(-y12.*z14+z12.*y14).*(x12.*y13-y12.*x13),Kyz)...
+kron(idetB.*(x13.*y14-y13.*x14).*(y12.*z13-z12.*y13),Kxz')...
+kron(idetB.*(-x12.*y14+y12.*x14).*(y12.*z13-z12.*y13),Kyz')...
+kron(idetB.*(y12.*z13-z12.*y13).*(x12.*y13-y12.*x13),Kzz);
dydz=kron(idetB.*(-x13.*z14+z13.*x14).*(x13.*y14-y13.*x14),Kxx)...
+kron(idetB.*(-x13.*z14+z13.*x14).*(-x12.*y14+y12.*x14),Kxy)...
+kron(idetB.*(-x13.*z14+z13.*x14).*(x12.*y13-y12.*x13),Kxz)...
+kron(idetB.*(x13.*y14-y13.*x14).*(x12.*z14-z12.*x14),Kxy')...
+kron(idetB.*(x12.*z14-z12.*x14).*(-x12.*y14+y12.*x14),Kyy)...
+kron(idetB.*(x12.*z14-z12.*x14).*(x12.*y13-y12.*x13),Kyz)...
+kron(idetB.*(x13.*y14-y13.*x14).*(-x12.*z13+z12.*x13),Kxz')...
+kron(idetB.*(-x12.*y14+y12.*x14).*(-x12.*z13+z12.*x13),Kyz')...
+kron(idetB.*(-x12.*z13+z12.*x13).*(x12.*y13-y12.*x13),Kzz);

```

Local postprocessing Once we have computed the solution $(\mathbf{q}_h, u_h, \hat{u}_h) \in \mathbf{V}_h \times W_h \times M_h$ for the HDG equations, we can use some of the known superconvergence property to justify why (for $k \geq 1$) the following local postprocessing is superconvergent. We compute

$$u_h^* \in \prod_{K \in \mathcal{T}_h} \mathcal{P}_{k+1}(K)$$

satisfying

$$\begin{aligned} (\nabla u_h^*, \nabla w_h)_K &= -(\kappa^{-1} \mathbf{q}_h, \nabla w_h)_K \quad \forall w_h \in \mathcal{P}_{k+1}(K), \\ (u_h^*, 1)_K &= (u_h, 1)_K. \end{aligned}$$

The HDG code provides decompositions:

$$u_h|_K = \sum_{j=1}^{d_3(k)} u_j^K P_j^K, \quad q_{\#,h}|_K = \sum_{j=1}^{d_3(k)} q_{\#,j}^K P_j^K$$

We then use the fact that

$$\int_K D_1^K D_i^K = 0 \quad \forall i \geq 2, \quad \forall K \in \mathcal{T}_h,$$

to decompose

$$u_h^*|_K = u_1^K P_1^K + \sum_{j=2}^{d_3(k+1)} w_j^K,$$

and write the system

$$\sum_{j=2}^{d_3(k+1)} \left(\int_K \nabla P_j^K \cdot \nabla P_i^K \right) w_j^K = - \sum_{\# \in \{x,y,z\}} \sum_{j=1}^{d_3(k)} \left(\int_K \kappa^{-1} P_i^K \partial_{\#} P_j^K \right) q_{\#,j}^K \quad i = 2, \dots, d_3(k+1).$$

Therefore, we only need to locally solve systems with the stiffness matrix (eliminating first row and columns) using variable convection matrices to build the right hand side. *This is the only place in the code where we explicitly use orthogonality properties of the polynomial basis.*

```
function uhstar=postprocessing(T,km,qhx,qhy,qhz,uh,k,formula)

% uhstar=postprocessing(T,km,qhx,qhy,qhz,uh,k,formula)
%
% Last modified: April 9, 2013

% Dimensions
d3plus=nchoosek(k+1+3,3);
d3=nchoosek(k+3,3);
Nelts=size(T.elements,1);

% Matrices
S=Stiffness(T,k+1,formula);
S(1,:,:)=[];
S(:,1,:)=[];
[Cx,Cy,Cz]=VariableConv(T,km,km,km,k+1,formula);
Cx=permute(Cx,[2 1 3]);
Cy=permute(Cy,[2 1 3]);
Cz=permute(Cz,[2 1 3]);
Cx(:,d3+1:end,:)=[];
Cy(:,d3+1:end,:)=[];
```

```

Cz(:, d3+1:end, :) = [];
Cx(1, :, :) = [];
Cy(1, :, :) = [];
Cz(1, :, :) = [];

% Solution of local problems

uhstar=zeros(d3plus-1,Nelts);
parfor K=1:Nelts
    uhstar(:,K)=-S(:, :, K) \ (Cx(:, :, K)*qhxc(:,K)+...
                                Cy(:, :, K)*qhyc(:,K)+...
                                Cz(:, :, K)*qhzc(:,K));
end
uhstar=[uh(1, :); uhstar];

```

14 Convection-difussion

The convection-diffusion equations are written as

$$\kappa^{-1} \mathbf{q} + \nabla u = 0, \quad \text{and} \quad \nabla \cdot (\mathbf{q} + u \boldsymbol{\beta}) + c u = f \quad \text{in } \Omega.$$

On the Neumann boundary, the condition is given as $-(\mathbf{q} + u \boldsymbol{\beta}) \cdot \boldsymbol{\nu} = \mathbf{u}_N \cdot \boldsymbol{\nu}$.

The local HDG equations are

$$\begin{aligned}
(\kappa^{-1} \mathbf{q}_h, \mathbf{r}_h)_K - (u_h, \nabla \cdot \mathbf{r}_h)_K + \langle \hat{u}_h, \mathbf{r}_h \cdot \boldsymbol{\nu} \rangle_{\partial K} &= 0 & \forall \mathbf{r}_h \in \mathbf{V}_h, \\
(\nabla \cdot \mathbf{q}_h, w_h)_K - (u_h, \boldsymbol{\beta} \cdot \nabla w_h)_K + (c u_h, w_h)_K \\
+ \langle \tau(u_h - \hat{u}_h) + (\boldsymbol{\beta} \cdot \boldsymbol{\nu}) \hat{u}_h, w_h \rangle_{\partial K} &= (f, w_h)_K & \forall w_h \in W_h.
\end{aligned}$$

The induced flux on the boundary is

$$\mathbf{q}_h \cdot \boldsymbol{\nu} + \tau(u_h - \hat{u}_h) + (\boldsymbol{\beta} \cdot \boldsymbol{\nu}) \hat{u}_h.$$

Most of the derivations are straightforward extensions of the pure diffusion problem. The local solvers contain the $4d_3 \times 4d_3 \times N_{\text{elt}}$ array

$$\mathbb{A}_1^K := \begin{bmatrix} M_{\kappa^{-1}}^K & \mathbf{O} & \mathbf{O} & -(C_x^K)^\top \\ \mathbf{O} & M_{\kappa^{-1}}^K & \mathbf{O} & -(C_y^K)^\top \\ \mathbf{O} & \mathbf{O} & M_{\kappa^{-1}}^K & -(C_z^K)^\top \\ C_x^K & C_y^K & C_z^K & M_c^K + \tau \mathbf{P} \mathbf{P}^K - \sum_{\star \in \{x,y,z\}} \beta_\star C_\star^K \end{bmatrix},$$

where $\beta_\star C_\star^K$ is the transpose of the variable convection matrix with entries

$$\int_K \beta_\star P_i^K \partial_x P_j^K \quad i, j = 1, \dots, d_3.$$

The $4d_3 \times 4d_2 \times N_{\text{elt}}$ array with slices

$$\mathbb{A}_2^K := \begin{bmatrix} (n_x \mathbf{D} \mathbf{P}^K)^\top \\ (n_y \mathbf{D} \mathbf{P}^K)^\top \\ (n_z \mathbf{D} \mathbf{P}^K)^\top \\ -(\tau \mathbf{D} \mathbf{P}^K)^\top + \sum_{\star \in \{x,y,z\}} (n_\star \beta_\star \mathbf{D} \mathbf{P}^K)^\top \end{bmatrix},$$

where $n_\star \beta_\star \mathbf{D} \mathbf{P}^K$ is the matrix with entries

$$\int_{e_\ell^K} \beta_\star \nu_\star D_i^{e_\ell^K} P_j^K \quad i = 1, \dots, d_2, \quad j = 1, \dots, d_3, \quad \ell \in \{1, 2, 3, 4\}.$$

The matrices \mathbb{A}_3^K and \mathbb{A}_f^K are the same as in the purely diffusive problem. Finally, the local solvers include the $4d_2 \times 4d_2 \times N_{\text{elt}}$ array with slices

$$\mathbb{C}^K := \mathbb{A}_3^K (\mathbb{A}_1^K)^{-1} \mathbb{A}_2^K + \tau \text{DD}^K - \sum_{\star \in \{x,y,z\}} n_{\star} \beta_{\star} \text{DD}^K,$$

where $n_{\star} \beta_{\star} \text{DD}^K$ has elements

$$\int_{e_\ell^K} \beta_{\star} \nu_{\star} D_i^{e_\ell^K} D_j^{e_\ell^K} \quad i, j = 1, \dots, d_2, \quad \ell \in \{1, 2, 3, 4\}.$$

The local solver related to source terms \mathbb{C}_f^K are defined with the same formulas as in the diffusive case. Everything else is taken verbatim from the diffusive HDG code.

```
function [C,Cf,A1,A2,Af]=localsolvers3dCD(km,c,f,beta,tau,T,k,formulas)

% [C,Cf,A1,A2,Af]=localsolvers3dCD(km,c,f,{betax,betay,betaz},...
%                               tau,T,k,{for1,for2,for3,for4})
%
%Input:
%   km, c, f: vectorized functions of three variables
%   {betax,betay,betaz}: vectorized functions of three variables
%   tau: penalization parameter for HDG (Nelts x 4)
%   T: expanded tetrahedrization
%   k: polynomial degree
%   for1: quadrature formula 3d (for mass matrix)
%   for2: quadrature formula 3d (for convection matrices)
%   for3: quadrature formula 2d
%   for4: quadrature formula 2d (variable coefficients and errors)
%
%Output:
%   C: 4*d2 x 4*d2 x Nelts
%   Cf: 4*d2 x Nelts
%   A1: 4*d3 x 4*d3 x Nelts
%   A2: 4*d3 x 4*d2 x Nelts
%   Af: 4*d3 x Nelts
%
%Last modified: April 11, 2013

Nelts=size(T.elements,1);
d2=nchoosek(k+2,2);
d3=nchoosek(k+3,3);

f=testElem(f,T,k,formulas{1});
Af=zeros(4*d3,Nelts);
Af(3*d3+1:4*d3,:)=f;

Mass=MassMatrix(T,{km,c},k,formulas{1});
Mk=Mass{1};Mc=Mass{2};
[Cx,Cy,Cz]=ConvMatrix(T,k,formulas{2});
[convx,convy,convz]=VariableConv(T,beta{1},beta{2},beta{3},k,formulas{1});
convbeta=permute(convx+convy+convz,[2 1 3]);

[tauPP,tauDP,nxDp,nyDP,nzDP,tauDD]=matricesFace(T,tau,k,formulas{3});
nx=T.normals(:, [1 4 7 10])';
ny=T.normals(:, [2 5 8 11])';
nz=T.normals(:, [3 6 9 12])';
bnDP=matricesVariableFaceA(T,beta,{nx,ny,nz},k,formulas{4});
bnDP=bnDP{1}+bnDP{2}+bnDP{3};
bnDD=matricesVariableFaceB(T,beta,{nx,ny,nz},k,formulas{4});
bnDD=bnDD{1}+bnDD{2}+bnDD{3};

O=zeros(d3,d3,Nelts);
```

```

A1=[Mk      ,O      ,O      ,-permute(Cx,[2 1 3]);...
    O      ,Mk      ,O      ,-permute(Cy,[2 1 3]);...
    O      ,O      ,Mk      ,-permute(Cz,[2 1 3]);...
    Cx      ,Cy      ,Cz      ,Mc+tauPP-convbeta];
A2=[permute(nxDP,[2 1 3]);...
    permute(nyDP,[2 1 3]);...
    permute(nzDP,[2 1 3]);...
    -permute(tauDP,[2 1 3])+permute(bnDP,[2 1 3])];

C=zeros(4*d2,4*d2,Nelts);
Cf=zeros(4*d2,Nelts);

parfor i=1:Nelts
    C(:, :, i)=[nxDP(:, :, i) nyDP(:, :, i) nzDP(:, :, i) tauDP(:, :, i)]/...
                A1(:, :, i)*A2(:, :, i)+tauDD(:, :, i)-bnDD(:, :, i);
    Cf(:, i) =[nxDP(:, :, i) nyDP(:, :, i) nzDP(:, :, i) tauDP(:, :, i)]/...
              A1(:, :, i)*Af(:, i);
end
return

```

```

function [Uh,Qxh,Qyh,Qzh,Uhat,system,solvers]=...
    HDG3dCD(km,c,f,beta,tau,T,k,formulas,uD,gx,gy,gz,varargin)

%[Uh,Qxh,Qyh,Qzh,Uhat]=HDG3dCD(km,c,f,{bx,by,bz},...
%                               tau,T,k,formulas,uD,gx,gy,gz)
%[Uh,Qxh,Qyh,Qzh,Uhat]=HDG3dCD(km,c,f,{bx,by,bz},...
%                               tau,T,k,formulas,uD,gx,gy,gz,0)
%[-,-,-,-,-,system,solvers]=HDG3dCD(km,c,f,{bx,by,bz},...
%                                     tau,T,k,formulas,uD,gx,gy,gz,1)
%
%
%Input:
%   km   : vectorized function (kappa^{-1}; kappa=diffusion parameter)
%   c    : vectorized function (reaction parameter)
%   f    : vectorized function (source term)
%   {bx,by,bz} : vectorized functions (convection field)
%   tau  : penalization parameter for HDG (Nelts x 4)
%   T    : expanded tetrahedrization
%   k    : polynomial degree
%   formulas: {for1,for2,for3,for4}
%            (quadrature formulas as used by localsolvers3dCD)
%   uD   : Dirichlet data; vectorized function
%   gx,gy,gz : Neumann data (corresponds to kappa*grad(u)); vectorized fns
%
%Output:
%   Uh    : d3 x Nelts,   matrix with uh
%   Qxh   : d3 x Nelts,   matrix with qxh
%   Qyh   : d3 x Nelts,   matrix with qyh
%   Qzh   : d3 x Nelts,   matrix with qzh
%   Uhat  : d2 x Nelts    matrix with uhhat
%   system : {HDGmatrix,HDGrhs,list of free d.o.f.,list of dir d.o.f.}
%   solvers : {A1,A2,Af}   local solvers
%
%Last modified: April 11, 2013

if nargin==13
    export=varargin{1};
else
    export=0;
end

d2=nchoosek(k+2,2);
d3=nchoosek(k+3,3);
block3=@(x) (1+(x-1)*d3):(x*d3);
Nelts =size(T.elements,1);
Nfaces=size(T.faces,1);

```

```

Ndir =size(T.dirichlet,1);
Nneu =size(T.neumann,1);

%Matrices for assembly process

face=T.facebyele'; % 4 x Nelts
face=(face(:)-1)*d2; % First degree of freedom of each face by element
face=bsxfun(@plus,face,1:d2); %4*Nelts x d2 (d.o.f. for each face)
face=reshape(face',4*d2,Nelts); %d.o.f. for the 4 faces of each element

[J,I]=meshgrid(1:4*d2);
R=face(I(:,:),:); R=reshape(R,4*d2,4*d2,Nelts);
C=face(J(:,:),:); C=reshape(C,4*d2,4*d2,Nelts);
% R.ij^K d.o.f. for local (i,j) d.o.f. in element K ; R.ij^K=C.ji^K
RowsRHS=reshape(face,4*d2*Nelts,1);

dirfaces=(T.dirfaces(:)-1)*d2;
dirfaces=bsxfun(@plus,dirfaces,1:d2);
dirfaces=reshape(dirfaces',d2*Ndir,1);

free=((1:Nfaces)-1)*d2;
free=bsxfun(@plus,free,1:d2);
free=reshape(free',d2*Nfaces,1);
free(dirfaces)=[];

neufaces=(T.neufaces(:)-1)*d2;
neufaces=bsxfun(@plus,neufaces,1:d2);
neufaces=reshape(neufaces',d2*Nneu,1);

%Local solvers and global system

[M1,Cf,A1,A2,Af]=localsolvers3dCD(km,c,f,beta,tau,T,k,formulas);
M=sparse(R(:),C(:),M1(:));
phif=accumarray(RowsRHS,Cf(:));

[uhatD,qhatN]=BC3d(uD,gx,gy,gz,T,k,formulas{3});

%Dirichlet BC
Uhatv=zeros(d2*Nfaces,1);
Uhatv(dirfaces)=uhatD; %uhat stored as a vector: d2*Nfaces

%RHS
rhs=zeros(d2*Nfaces,1);
rhs(free)=phif(free);
qhatN=reshape(qhatN,d2*Nneu,1); % qhatN stored as a vector: d2*Nneu
rhs(neufaces)=rhs(neufaces)+qhatN;
rhs=rhs-M(:,dirfaces)*Uhatv(dirfaces);

if export
    system={M,rhs,free,dirfaces};
    solvers={A1,A2,Af};
    Uh=[];
    Qxh=[];
    Qyh=[];
    Qzh=[];
    Uhat=[];
    return
else
    system=[];
    solvers=[];
end

Uhatv(free)=M(free,free)\rhs(free);
Uhat=reshape(Uhatv,d2,Nfaces);

%Uh Qxh Qyh Qzh

```

```

faces=T.facebyele'; faces=faces(:);
uhhataux=reshape(Uhat(:,faces),[4*d2,Nelts]);
sol=zeros(4*d3,Nelts);
parfor K=1:Nelts
    sol(:,K)=A1(:, :,K)\(Af(:,K)-A2(:, :,K)*uhhataux(:,K));
end

Qxh=sol(block3(1),:);
Qyh=sol(block3(2),:);
Qzh=sol(block3(3),:);
Uh =sol(block3(4),:);
return

```

15 Quadrature rules

The scripts and `TableQuadForm.m` include `TablesQuadForm3d.m` matrices with quadrature formulas in the reference elements in two and three dimensions respectively. They are stored as $N_{qd} \times 5$ matrices in the three dimensional case and as $N_{qd2} \times 4$ matrices in the two dimensional case. The collection of formulas that are stored in those files is given in Tables 1 and 2. Once the polynomial degree k is chosen, the function `checkQuadrature3d` chooses formulas for all two and three dimensional integrals. We avoid using the two dimensional quadrature formulas that use nodes on the edges of the reference triangle.

name	degree of precision	number of quadrature nodes = N_{qd}
tetra1	1	1
tetra3	2	4
tetra5	5	14
tetra7	6	25
tetra9	8	45

Table 1: Quadrature formulas on \hat{K}

name	degree of precision	number of nodes N_{qd2}	nodes on edges
matrix0	1	1	No
matrix2	2	3	No
matrix4	4	6	No
matrix5	5	10	Yes
matrix7	7	15	Yes
matrix9	9	21	No
matrix11	11	28	Yes
matrix13	13	36	No
matrix14	14	45	Yes
matrix16	16	55	Yes
matrix18	18	66	No
matrix20	20	78	No
matrix21	21	91	No
matrix23	23	105	No
matrix25	25	120	Yes

Table 2: Quadrature formulas on \hat{K}_2

```

function formulas=checkQuadrature3d(k,constantmass)

```

```

%formulas=checkQuadrature3d(k,constantmass)
%Imput:
%           k: degree of polynomials
%   constantmass: 1 constant coefficients in mass matrices
%                 0 non-constant
%Output:
%   formulas{1} : 3d quadrature formula for errors and var coeff
%   formulas{2} : 3d quadrature formula for constant coefficients
%   formulas{3} : 2d quadrature formula
%   formulas{4} : 2d quadrature formula for errors
%Last update: March 14, 2013

% degrees = {3k,2k,2k,2k+2} if constant mass = 0
%           {2k,2k,2k,2k+2} if constant mass = 1
% for k=0, take {2,0,0,2}

TablesQuadForm3d
TablesQuadForm
switch constantmass
    case 1
        switch k
            case 0
                formulas={tetra5,tetra1,matrix0,matrix4};
            case 1
                formulas={tetra3,tetra3,matrix4,matrix4};
            case 2
                formulas={tetra7,tetra7,matrix9,matrix9};
            case 3
                formulas={tetra9,tetra9,matrix11,matrix11};
        end
    case 0
        switch k
            case 0
                formulas={tetra5,tetra1,matrix0,matrix4};
            case 1
                formulas={tetra5,tetra3,matrix4,matrix4};
            case 2
                formulas={tetra7,tetra7,matrix9,matrix9};
            case 3
                formulas={tetra9,tetra9,matrix11,matrix11};
        end
    end
formulas{3}(:,4)=formulas{3}(:,4)/2;
formulas{4}(:,4)=formulas{4}(:,4)/2;
return

```

16 Main programs and their dependences

Routines needed to start working. Note that implementation of the Dubiner polynomials in two dimensions uses code for the Jacobi polynomials as a subfunction. This has been adapted from a piece of code by John Burkardt, distributed under the GNU LGPL license. Quadrature rules have been pre-stored in the form that is needed for the code. Instead of having an m-file with the formulas, there is a script that defines them one by one, and a function that chooses the ones that are going to be used for a given polynomial degree. This is done only once, so this part of the code can be easily modified. The three dimensional formulas that have been included can deal with all cases up to $k = 3$. For higher order, one can easily construct more formulas and modify the corresponding files.

- HDGgrid3d
- createTau3d

- checkQuadrature3d
 - TablesQuadFrom3d
 - TablesQuadForm

Main functions.

- HDG3d
 - localsolvers3d
 - * MassMatrix
 - dubiner3d
 - * ConvMatrix
 - dubiner3d
 - * matricesFace
 - dubiner2d
 - dubiner3d
 - BC3d
 - * dubiner2d
- HDG3dCD
 - localsolvers3dCD
 - * MassMatrix
 - dubiner3d
 - * ConvMatrix
 - dubiner3d
 - * VariableConv
 - dubiner3d
 - * matricesVariableFaceA
 - dubiner2d
 - dubiner3d
 - * matricesVariableFaceB
 - dubiner2d
 - BC3d
 - * dubiner2d

Projections and error functions for testing

- L2proj3d
 - dubiner3d
 - errorElem
 - * dubiner3d
- L2projskeleton3d
 - dubiner2d
 - errorFaces
 - * dubiner2d

- projectHDG3d
 - MassMatrix
 - * dubiner3d
 - matricesFace
 - * dubiner2d
 - * dubiner3d
 - testElem
 - * dubiner3d
 - testFaces
 - * dubiner2d
- errorElem
 - dubiner3d
- errorFaces
 - dubiner2d
- postprocessing
 - variableConv
 - * dubiner3d
 - Stiffness
 - * dubiner3d

17 Alphabetical list of all programs

Main programs.

- BC3d
- checkQuadrature3d
- ConvMatrix
- createTau3d
- dubiner2d
- dubiner3d
- errorElem
- errorFaces
- HDG3d
- HDG3dCD
- HDGgrid3d
- L2proj3d
- L2projskeleton3d

- localsolvers3d
- localsolvers3dCD
- MassMatrix
- matricesFace
- matricesVariableFaceA
- matricesVariableFaceB
- postprocessing
- projectHDG3d
- Stiffness
- TablesQuadForm
- TablesQuadForm3d
- testElem
- testFaces
- VariableConv

Examples of fully developed meshes

- 4Tchimney
- Corner
- FicheraCorner1
- FicheraCorner2
- sixT3dDir

Scripts

- Script_HDG3DCD
- scriptHDG3dpaper