

HDG scheme to eigenvalues of poisson equation

Un método de Galerkin Discontinuo Hibridizable para la ecuación de Schrödinger estacionaria lineal

Resultados preliminares de @alujan

```
clear
format short
syms x y z real
```

```
% Let's add to the path the src and drivers: Original Article
addpath('/Users/chubbs/Documents/UN/Schrodinger/MATLAB/949_Sayas/Matlab/
Drivers/')
addpath('/Users/chubbs/Documents/UN/Schrodinger/MATLAB/949_Sayas/
Matlab/Src/')

% Let's add the path of the gmsh structure: Load Mesh structure
addpath('/Users/chubbs/Documents/UN/Schrodinger/MATLAB/gmsh/')

% Let's add the path of the structures created: Spectral definitions
addpath('/Users/chubbs/Documents/UN/Schrodinger/MATLAB/spectral/mesh/')
addpath('/Users/chubbs/Documents/UN/Schrodinger/MATLAB/spectral/src/')
```

0. Preliminaries

Load of structures and previous definitions.

Load of structures for analisys

Let's load the reference structures we're going to use to set the pilot example

```
% Importing of a singular structure for first case scenario: Unitary cube
T = load_mesh('pi-cubeD4.msh')
```

```
T = struct with fields:
  coordinates: [4748x3 double]
  elements: [22770x4 double]
  dirichlet: [4132x3 double]
  neumann: [0x3 double]
  faces: [47606x4 double]
  dirfaces: [43475 43476 43477 43478 43479 43480 43481 43482 43483 43484 43485 43486 43487 43488 43489]
  neufaces: [1x0 double]
  facebyele: [22770x4 double]
  orientation: [22770x4 double]
  perm: [22770x4 double]
  volume: [22770x1 double]
  area: [47606x1 double]
  normals: [22770x12 double]
```

```
% Listing of elements for growth of method testing
listT = {T};
```

1. Construction of the scheme

Definition of the equation and the main elements needed to interact and create the solutions.

Definitions of reference solutions

First let's define the values we're going to compare with, in this case the functions u and q , defined for the auxiliar equation, it's important to notice that for instance ψ corresponds to the wave function of the particle and J to the complex conjugate of the kinetic momentum operator applied to the wave function

$$\nabla u(r) + q(r) = 0 \text{ in } \Omega$$

$$-\operatorname{div} q(r) = \lambda u(r) \text{ in } \Omega$$

$$u(r) = 0 \text{ on } \partial\Omega$$

Take in mind this a scalar PDE, for this scenario every evaluation of the values must be in components of the vector.

```
% Let's define a simple value for U: harmonic vector
% - Characteristics of the function in space
U(x, y, z) = sin(x)*sin(y)*sin(z)
```

```
U(x, y, z) = sin(x) sin(y) sin(z)

% Partial derivarives of the component
Ux = diff(U, x); Uxx = diff(U, x, 2);
Uy = diff(U, y); Uyy = diff(U, y, 2);
Uz = diff(U, z); Uzz = diff(U, z, 2);

Q = -[Ux; Uy; Uz] % Gradient definition
```

$$Q(x, y, z) = \begin{pmatrix} -\cos(x) \sin(y) \sin(z) \\ -\cos(y) \sin(x) \sin(z) \\ -\cos(z) \sin(x) \sin(y) \end{pmatrix}$$

```
% Definition of potential taking action
F(x, y, z) = - (Uxx + Uyy + Uzz)
```

$$F(x, y, z) = 3 \sin(x) \sin(y) \sin(z)$$

```
% Processing of functions
u = matlabFunction(U, Vars={x, y, z});

qx = matlabFunction(-Ux, Vars={x, y, z});
qy = matlabFunction(-Uy, Vars={x, y, z});
qz = matlabFunction(-Uz, Vars={x, y, z});
```

```
% Validation of dirichlet condition
```

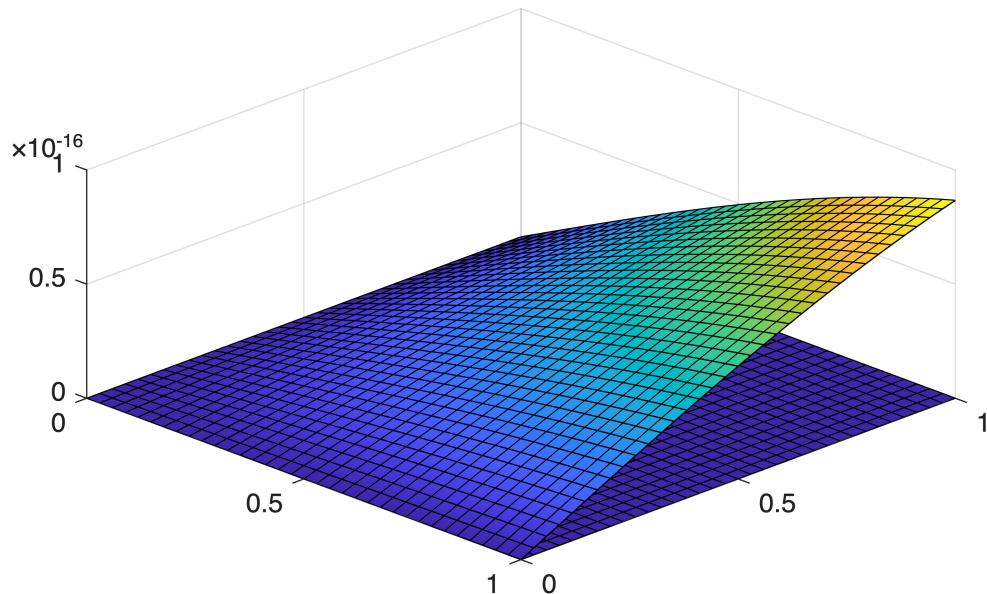
```

clf('reset')

% Plot of conditions Null conditions for psi {x, y, z}
fig = figure; theme(fig,"auto");
hold on
fsurf(@(x, y) u( x,     y,     0), [0 1 0 1])      % Condition for z = 0
fsurf(@(x, y) u( x,     y, pi), [0 1 0 1])        % Condition for z = pi
fsurf(@(x, z) u( x,     0,     z), [0 1 0 1])        % Condition for y = 0
fsurf(@(x, z) u( x, pi,     z), [0 1 0 1])        % Condition for y = pi
fsurf(@(y, z) u( 0,     y,     z), [0 1 0 1])        % Condition for x = 0
fsurf(@(y, z) u( pi,     y,     z), [0 1 0 1])       % Condition for x = pi

hold off
grid on
view([45, 45])

```



Definition of Cuadrature and Polynomial degrees

Now for the first definitions for the method, we must import the cuadrature that's going to be used, and the polynomial degree that's going to be used for the solution

```

% It's possible to change the values below to alter the polynomial and
% cuadrature precision for more general viewing
TablesQuadForm3d          % Importing of cuadrature for thetetrahedron
TablesQuadForm              % Importing of cuadrature for triangles

k = 2; % Polynomial Degree

% Switch case for the selection of formulas: cuadratures
switch k
    case 0

```

```

        formulas={tetra3,tetra1,matrix0,matrix4};
case 1
    formulas={tetra5,tetra3,matrix4,matrix9};
case 2
    formulas={tetra7,tetra5,matrix9,matrix11};
case 3
    formulas={tetra9,tetra7,matrix11,matrix14};
case 4
    formulas={tetra9,tetra9,matrix14,matrix16};
end

% Reduction of weights: Sum of weights it's defined to be equal to 2, for
% normalization it's reduced to 1.
formulas{3}(:,4)=formulas{3}(:,4)/2;
formulas{4}(:,4)=formulas{4}(:,4)/2;

```

Norm of solutions for error definitions

The errorElem function it's used for this task, the idea used it's comparison with the origin that leaves the norm of elements u and q with known solution

$$|\mathbf{p} - \mathbf{p}^*|_{L^2} = |\mathbf{p}|_{L^2} : \mathbf{p}^* = 0$$

```

% Error elements definition for display handle
ErrorU      =[];
ErrorQ      =[];
ErrorUhat   =[];
ErrorLambda =[];

ErrorPu     =[];
ErrorPuhat =[];
ErrorUstar  =[];
h          =[];

```

```

% Norms of unknowns for relative error
Tmax=listT{end};                      % Listing of T elements
Nelts=size(T.elements,1);               % Number of elements enlisted
d3=nchoosek(k+3,3);                   % d_i definition of set (cardinality)

```

2. Scheme definition

Definition of the main iteration, mesh elements and bilinear forms

HDG: The main iteration

Firstly the method it's created to run in a single run (*presence of one element only*), with this in mind, when going to expand the idea must be iterated over the different structures

```

% Definition of the action of tau: Identity
tau = 1*ones(4,Nelts);

% ----- HDG 3D main function
----- %

% Definitions asociated with the tetrahedrization
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);

% 4th intervention
% - Faces
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_d2 = face(I(:, :)); R_d2=reshape(R_d2,4*d2,4*d2,Nelts); % Mesh grid
% definition inside T_i element "Row-Axis"
C_d2 = face(J(:, :)); C_d2=reshape(C_d2,4*d2,4*d2,Nelts); % Mesh grid
% definition inside T_i element "Column-Axis"

% - Volumes
element = (1:Nelts); % Nelts
element = (element(:)-1)*4*d3; % First degree of freedom of
% each face by element
element = bsxfun(@plus,element,1:4*d3); % 4*Nelts x d2 (d.o.f. for
% each face)
element = reshape(element',4*d3,Nelts); % d.o.f. for the 4 faces of
% each element

[J,I] = meshgrid(1:4*d3);

R_d3 = element(I(:, :)); R_d3 = reshape(R_d3,4*d3,4*d3,Nelts); % Mesh grid
% definition inside T_i element "Row-Axis"
C_d3 = element(J(:, :)); C_d3 = reshape(C_d3,4*d3,4*d3,Nelts); % Mesh grid
% definition inside T_i element "Column-Axis"

```

```

% R_ij^K d.o.f. for local (i,j) d.o.f. in element K ; R_ij^K=C_ji^K
RowsRHS_d2 = reshape(    face,4*d2*Nelts,1); % Definition of
solution shape
RowsRHS_d3 = reshape(element,4*d3*Nelts,1); % Definition of
solution shape

% 4th intervention
% Dirichlet faces: defintion
dirfaces = (T.dirfaces(:)-1)*d2; % First degree of freedom of each
face by element
dirfaces = bsxfun(@plus,dirfaces,1:d2); % Bitwise sum of dirfaces and
1:d2 > dirfaces + 1:d2
dirfaces = reshape(dirfaces',d2*Ndir,1); % Reshape of dirfaces

% Reduced version of free
free = (1: d2*Nfaces);

% Cleaning of dirfaces: Positions not needed
free(dirfaces) = []; % Empty of dirfaces positions on free

% Neumann faces: defintion
neufaces = (T.neufaces(:)-1)*d2; % First degree of freedom of each
face by element
neufaces = bsxfun(@plus,neufaces,1:d2); % Bitwise sum of neufaces and
1:d2 > neufaces + 1:d2
neufaces = reshape(neufaces',d2*Nneu,1);

% Reordering of values find indexes
indexes = arrayfun(@(i) find(T.facebyele == T.dirfaces(i)),
1:size(T.dirfaces, 2));

% - Map of values indexes
map = T.orientation(indexes) == -1; T.faces(T.dirfaces(map), [2 3]) =
T.faces(T.dirfaces(map), [3 2]);

% Correction of orientation
T.orientation(indexes) = 1;

```

Now it's the point to use the local solvers, here are defined the change of basis and the change on the matrices for calculations needed.

```

% ----- Local solvers definition function
----- %

% Computation of the differentials form Matrix: Return in the already
desired form

% - Computation of Convection Integrals
[CMx, CMy, CMz] = ConvMatrix(T,k,formulas{1});

```

```

% - Computation of the Mass Integrals
Mass = MassMatrix(T,{@(x, y, z) 0*x.*y.*z + 1, @(x, y, z) 0*x},
k,formulas{1});
% - ALR: Reduce this computation into one single line
Mi=Mass{1};

% - Computation of Faces Integrals
[tauPP,tauDP,nxDP,nyDP,nzDP,tauDD]=matricesFace(T,tau,k,formulas{3});

% Condensation of matrices known
nDP = [nxDP, nyDP, nzDP]; divPP = [CMx, CMy, CMz];

% - Matrices defintions: A solvers local
A1=zeros(4*d3,4*d3,Nelts); % Solver storage reservation
A2=zeros(4*d3,4*d2,Nelts); % Solver storage reservation
A3=zeros(4*d3,4*d3,Nelts); % Solver storage reservation
A4=zeros(4*d2,4*d3,Nelts); % Solver storage reservation

% Matrices related to solvers
% - Definition of the Mass matrix asociated with a_1: 6*d3 x 6*d3
O = zeros(d3,d3,Nelts); % Big O cero matrix: Shapes juntions

% - Block definition of matrix
Mk = [Mi ,0 ,0 ; ...
       0 ,Mi ,0 ; ...
       0 ,0 ,Mi ];

A1 = [      Mk, -permute(divPP, [2 1 3]); ...
        divPP, tauPP      ];

% - Definition of the Mass matrix asociated with a_2: 6*d3 x 2*(4*d2)
% Pendiente la revisión de errores propuesta
A2 = [-permute(nDP , [2 1 3]) ; ...
        permute(tauDP, [2 1 3]) ];

O = zeros(3*d3,3*d3,Nelts); % Big O cero matrix: Shapes juntions
Ov = zeros(3*d3,d3,Nelts);

A3_w = [      Mk, 0v; ...
           permute(Ov, [2 1 3]), Mi];

A3 = [      0, 0v; ...
           permute(Ov, [2 1 3]), Mi];

O = zeros(d3,d3,Nelts); Ov = [0, 0, 0]; % Big O cero matrix: Shapes juntions

A4 = [Mk ,permute(Ov, [2, 1, 3]) ; ...
       Ov ,tauPP      ];

```

```

0 = zeros(4*d2,d3,Nelts);
A5 = [0, 0, 0, tauDP];

% Matrices definitions: C solvers Flux
CM = zeros(4*d2,4*d2,Nelts); % Solver storage reservation
CK = zeros(4*d2,4*d2,Nelts); % Solver storage reservation

% Operator definition
Q_w_U_w = zeros(4*d3, 4*d3, Nelts); % Solver operator storage reservation

Q_w      = zeros(4*d3, 4*d3, Nelts); % Solver Q_w storage reservation
U_w      = zeros(4*d3, 4*d3, Nelts); % Solver U_w storage reservation

% Parallel creation of flux operators
% Revisión del sistema final a generar
% - Element separation block
block_3d3 = [block3(1) block3(2) block3(3)];

parfor i=1:Nelts
    CM(:,:,i) = A2(:, :, i)' * (A1(:, :, i)' \ A4(:, :, i)) * (A1(:, :, i)
    \ A2(:, :, i)) - ...
                A2(:, :, i)' * (A1(:, :, i)' \ A5(:, :, i)') - ...
                A5(:, :, i) * (A1(:, :, i) \ A2(:, :, i)) + tauDD(:, :, i);
    CK(:,:,i) = A2(:, :, i)' * (A1(:, :, i)' \ A3(:, :, i)) * (A1(:, :, i)
    \ A2(:, :, i));
    Q_w_U_w(:, :, i) = A1(:, :, i) \ A3_w(:, :, i);
end

% Separation of operators
U_w(block3(4),block3(4), :) = Q_w_U_w(block3(4), block3(4), :);
Q_w(block_3d3,block_3d3, :) = Q_w_U_w(block_3d3, block_3d3, :);

```

```

% Recovery of all elements
M = sparse(R_d2(:,C_d2(:), CM(:)); K = sparse(R_d2(:, C_d2(:),CK(:));

% Boundary conditions evaluation
% The resulting terms are:
% - uhartD : Reference term evaluation on the Dirichlet faces
% - qhatN : Reference term evaluation on the Neumann faces
[etahatD, qhatN] = BC3d(@(x, y, z) 0*x,@(x, y, z) 0*x,@(x, y, z) 0*x,@(x,
y, z) 0*x,T,k,formulas{3});

% Dirichlet BC: Storage
etahatD=reshape(etahatD,d2*Ndir,1); % uhatD stored as a vector: (2*d2*Ndir)
x 1 : todo > Adjust space
Etahatv=zeros(d2*Nfaces, 1); % Storage reservation

```

```

Etahatv(dirfaces)=etahatD;           % Uhat stored as a vector: d2*Nfaces
Etahatv(free) = 1;

% Export of the system
system={M, K, free, dirfaces};
solvers={A1, A2, A3, A4, A5};
Uh=[]; Qxh=[]; Qyh=[]; Qzh=[]; Uhat=[];

% RHS currently has the information of the frontier conditions
% and the information of inner skeleton: solution of uhat
numEig = 1;

% [Etav_free, lambda] = eigs(M, K, numEig, 1E-5); lambda = diag(lambda)';
[Etav_free, lambda] = eigs(M(free, free), K(free, free), numEig, 1E-2);
lambda = diag(lambda)'

lambda =
3.0019e+00

```

```

% % Insertion of BC
Etav = zeros(d2*Nfaces, numEig);
Etav(dirfaces, :) = repmat(etahatD, 1, numEig);
Etav(free, :) = Etav_free - M(free,dirfaces)*Etav(dirfaces, :);

% Reorganization of values
Eta=zeros(d2, Nfaces, numEig);

Uh=zeros(d3,Nelts, numEig);                      % Reservation
of storage

Qxh=zeros(d3,Nelts, numEig);                     % Reservation
of storage
Qyh=zeros(d3,Nelts, numEig);                     % Reservation
of storage
Qzh=zeros(d3,Nelts, numEig);                     % Reservation
of storage

sol = zeros(4*d3, 1);                            % Temporal
reservation of space

maxIter = 0;                                     % Max
iterations / distance permitted

delta = 1E-5;

% Parallel solution of system: Newton algorithm
for N = 1:numEig

    % Reordering of faces
    Eta_n = reshape(Etav(:, N), [d2, Nfaces]);

```

```

% Assignment of variables
Etav_n = Etav(:, N);

% Energies found
lambda_0 = lambda(N); lambda_n = lambda_0;

% Tolerance till convergence
tolerance = 1E-5; delta_refinement = 1E-3;

scale = 1; delta_lambda = 1;

for iter=1:maxIter

    % Reordering of faces
    Eta_n = reshape(Etav_n, [d2, Nfaces]);

    % Normalization of input
    Eta_n = Eta_n / sqrt(inner_Face_L2(T,Eta_n,Eta_n,k,formulas{4}));

    % Computing of Linear form N
    CN_lambda = zeros(4*d2,4*d2,Nelts);           % Solver storage
reservation
    CM_lambda = zeros(4*d2,4*d2,Nelts);           % Solver storage
reservation

    for i = 1:Nelts
        % Reconstruction of faces bilinear form
        CN_lambda(:,:,:,i) = A2(:,:,i)' * (A1(:,:,i))' \ A3(:,:,i))
* ((eye(4*d3, 4*d3) - lambda_n * U_w(:,:,i))^2 \ (A1(:,:,i) \ A2(:,:,i)));
        CM_lambda(:,:,:,i) = A2(:,:,i)' * (A1(:,:,i))' \ A3(:,:,i))
* ((eye(4*d3, 4*d3) - lambda_n * U_w(:,:,i))^1 \ (A1(:,:,i) \ A2(:,:,i)));
    end

    % Projection into faces form
    N_lambda = sparse(R_d2(:,C_d2(:), CN_lambda(:)); M_lambda =
sparse(R_d2(:,C_d2(:), CM_lambda(:));

    % New eta iteration
    Etav_hat = (M - lambda_n * M_lambda) \ N_lambda * Etav_n;

    % Reordering of faces
    Eta_hat = reshape(Etav_hat, [d2, Nfaces]);

    % Normalization of input
    Eta_hat = Eta_hat /
sqrt(inner_Face_L2(T,Eta_hat,Eta_hat,k,formulas{4}));

```

```

% Normalization condition
Eta_L2_norm = inner_Face_L2(T,Eta_hat, Eta_n,k,formulas{4});

delta_lambda = 1 / Eta_L2_norm;

% Eta refinement criterion
if delta_refinement > abs(abs(delta_lambda) - 1)
    scale = abs(lambda_0 - lambda_n)/(lambda_0 - lambda_n) *
abs(scale)/2;
end

% Update value
lambda_n_1 = lambda_n + scale * delta_lambda; Etav_n = delta_lambda
* Etav_hat;

% Differences
epsilon = lambda_n_1 - lambda_n; lambda_n = lambda_n_1;

% Eta convergence criterion
if tolerance > abs(abs(delta_lambda) - 1); break; end

end

% Update of Eta
% - Reordering of faces
Eta_n = reshape(Etav_n, [d2, Nfaces]);

% - Recover of values per elements
faces = T.facebyele'; faces=faces(:); % Recovery of faces information
eta_aux = reshape(Eta_n(:, faces, :),[4*d2, Nelts]); % Reshape on the faces of Uhat

% Update of energies
lambda(N) = lambda_n;

% Exit variable of parfor
Eta(:,:, N) = Eta_n;

% Reconstruction of solution per energy
for i = 1:Nelts

    % Reconstruction of solution
    sol = A1(:,:,i)\A2(:,:,i) * eta_aux(:,:,i);

    % Fill of spaces
    % Version pasada:
    % Uh(:,:,i,N) = eye(d3, 4*d3) * ((eye(4*d3, 4*d3) - lambda_n *
U_w(:,:, i)) \ sol(:,:,i));

```

```

temporal = (eye(4*d3, 4*d3) - lambda_n * U_w(:, :, i)) \ sol(:, );

Uh(:,i,N) = temporal(block3(4));

Qxh(:,i,N) = sol(block3(1)) + lambda_n * Q_w(block3(1), block3(1),
i) * Uh(:,i,N);
Qyh(:,i,N) = sol(block3(2)) + lambda_n * Q_w(block3(2), block3(2),
i) * Uh(:,i,N);
Qzh(:,i,N) = sol(block3(3)) + lambda_n * Q_w(block3(3), block3(3),
i) * Uh(:,i,N);
end

end

lambda

```

```

lambda =
3.0019e+00

```

Error comparison with solution

Now we can review our process checking if the error obtained for the process done. Let's check the associated errors.

```

% Selection of n value to approximate
lambda_value = 1;

% Norms definitions
normU=errorElem(Tmax,u,zeros(d3,size(Tmax.elements, 1)),k,formulas{1});

normQ=errorElem(Tmax,qx,zeros(d3,size(Tmax.elements, 1)),k,formulas{1})...
+errorElem(Tmax,qy,zeros(d3,size(Tmax.elements, 1)),k,formulas{1})...
+errorElem(Tmax,qz,zeros(d3,size(Tmax.elements, 1)),k,formulas{1});

normEta = errorFaces(Tmax,u,zeros(d2,size(Tmax.faces, 1)),k,formulas{4});

% Errors with exact solution
error_eta = errorFaces(T, u, Eta(:, :, lambda_value), k, formulas{4});
error_q_ = errorElem (T, qx, Qxh(:, :, lambda_value), k, formulas{1})...
+ errorElem (T, qy, Qyh(:, :, lambda_value), k, formulas{1})...
+ errorElem (T, qz, Qzh(:, :, lambda_value), k, formulas{1});
error_u_ = errorElem (T, u, Uh(:, :, lambda_value), k, formulas{1});

error_eta_ = errorFaces(T, u, -Eta(:, :, lambda_value), k, formulas{4});
error_q_ = errorElem (T, qx, -Qxh(:, :, lambda_value), k, formulas{1})...
+ errorElem (T, qy, -Qyh(:, :, lambda_value), k, formulas{1})...
+ errorElem (T, qz, -Qzh(:, :, lambda_value), k, formulas{1});
error_u_ = errorElem (T, u, - Uh(:, :, lambda_value), k, formulas{1});

error_eta = min([error_eta, error_eta_]);
error_u_ = min([error_u_, error_u_]);

```

```
error_q = min([ error_q, error_q_]);
```

```
ErrorQ=[ErrorQ error_q/normQ]
```

```
ErrorQ = 1x4  
4.4831e-01 4.0437e-01 4.0319e-01 4.0080e-01
```

```
ErrorU=[ErrorU error_u/normU]
```

```
ErrorU = 1x4  
7.4212e-02 4.3511e-03 8.3333e-04 1.2529e-04
```

```
ErrorUhat=[ErrorUhat error_eta/normEta]
```

```
ErrorUhat = 1x4  
1.0987e-01 2.1048e-02 6.9546e-03 8.4642e-04
```

```
ErrorLambda = [ErrorLambda abs((3) - lambda(lambda_value)) / (33)]
```

```
ErrorLambda = 1x4  
1.4000e-03 6.5177e-04 2.1821e-04 5.7929e-05
```

```
% Rate of sucesion: Convergence verification
```

```
rateQ = log2(ErrorQ(1:end-1)./ErrorQ(2:end));  
rateU = log2(ErrorU(1:end-1)./ErrorU(2:end));  
rateEta = log2(ErrorUhat(1:end-1)./ErrorUhat(2:end));  
rateLambda = log2(ErrorLambda(1:end-1)./ErrorLambda(2:end));
```

```
% Display sequence of values
```

```
format bank  
disp('Rate |U-Uh|      Rate |U-Uhat|_h');
```

```
Rate |U-Uh|      Rate |U-Uhat|_h
```

```
disp([rateU' rateEta' rateLambda']);
```

```
4.09          2.38          1.10  
2.38          1.60          1.58  
2.73          3.04          1.91
```

```
format shortE
```

```
disp('Error |U-Uh|      Error |U-Uhat|_h');
```

```
Error |U-Uh|      Error |U-Uhat|_h
```

```
disp([ErrorU' ErrorUhat' ErrorLambda']);
```

```
7.4212e-02 1.0987e-01 1.4000e-03  
4.3511e-03 2.1048e-02 6.5177e-04  
8.3333e-04 6.9546e-03 2.1821e-04  
1.2529e-04 8.4642e-04 5.7929e-05
```