3D Vertex Model :: infinite sheet of cells

Initialization

In[ ]:=
```
NotebookDirectory[]
```

Out[ ]=
```
D:\LocalData\hashmial\3D vertex model - github\curved monolayer\
```

importing mesh

mesh parameters and specifying precision

In[ ]:=
```
(*DumpGet["C:\\Users\\aliha\\Desktop\\optimize.mx"];*)
DumpGet["D:\\LocalData\\hashmial\\3D vertex model - github\\curved
    monolayer\\create monolayer - smooth\\smoothgeometry.mx"];
ptsToIndAssoc = KeyMap[SetPrecision[#, 8] &, ptsToIndAssoc];
indToPtsAssoc = SetPrecision[#, 8] & /@ indToPtsAssoc;
wrappedMat = SetPrecision[#, 8] & /@ wrappedMat;
faceListCoords = SetPrecision[#, 8] & /@ faceListCoords;
yLim = yLim - yLim[[1]];
```

In[ ]:=
```
Names["Global`*"]
```

Out[ ]=
```
{cellVertexGrouping, edges, faceListCoords,
 indToPtsAssoc, ptsToIndAssoc, vertexToCell, wrappedMat, xLim, yLim}
```

In[ ]:=
```
Needs["CompiledFunctionTools`"];
```

call dependencies/misc

Launch IGraphM

In[ ]:=
```
Needs["IGraphM`"]
```

Out[ ]=
```
IGraph/M 0.5.1 (October 12, 2020)
Evaluate IGDocumentation[] to get started.
```

Launch Subkernels for parallel processing

In[∘]:=
```
LaunchKernels[]
ParallelTable[$KernelID, {i, $KernelCount}]
```

Out[∘]=
```
{KernelObject[ Name: Local kernel KernelID: 1 ], KernelObject[ Name: Local kernel KernelID: 2 ],
 KernelObject[ Name: Local kernel KernelID: 3 ], KernelObject[ Name: Local kernel KernelID: 4 ],
 KernelObject[ Name: Local kernel KernelID: 5 ], KernelObject[ Name: Local kernel KernelID: 6 ]}
```

Out[∘]=
```
{6, 5, 4, 3, 2, 1}
```

simulation variables and parameters

In[∘]:=
```
ClearAll[paramFinder];
Options[paramFinder] = {"OrientedFaces" → False};
paramFinder::OrientedFaces =
  "the option should be set to True if the faces of the cell
    are arranged in c.c.w direction.
Default
    →
    False";
```

In[∘]:=
```
SetOptions[paramFinder, "OrientedFaces" → True]
```

Out[∘]=
```
{OrientedFaces → True}
```

simulation parameters

In[∘]:=
```
time = δt = 0.005; (*time params*)
ϵcc = 1.; ϵco = 0.7; (*params for surface tension*)
kcv = 14.0;
Vo = 0.528187;(*volume elasticity and equilibrium volume*)
(*Vo=1.0;*)
Vgrowth = 1.0 × 10^-3; (*volume growth-rate*)
δ = 1.0 × 10^-3; (*length threshold for topological transitions*)
growingcellIndices = {⋯} + ;
```

In[∘]:=
```
ClearAll[orderlessHead];
SetAttributes[orderlessHead, {Orderless}];
```

simulation domain

In[•]:=
```
𝒟 = Rectangle[{First@xLim, First@yLim}, {Last@xLim, Last@yLim}];
```

local topological information

In[•]:=
```
periodicRules::Information =
  "shift the points outside the simulation domain to inside the domain";
transformRules::Information =
  "vector that shifts the point outside the simulation domain back inside";
Clear@periodicRules;
With[{xlim1 = xLim⟦1⟧, xlim2 = xLim⟦2⟧, ylim1 = yLim⟦1⟧, ylim2 = yLim⟦2⟧},
  periodicRules = Dispatch[{
     {x_ /; x ≥ xlim2, y_ /; y ≤ ylim1, z_} :→ SetPrecision[{x - xlim2, y + ylim2, z}, 8],
     {x_ /; x ≥ xlim2, y_ /; ylim1 < y < ylim2, z_} :→ SetPrecision[{x - xlim2, y, z}, 8],
     {x_ /; xlim1 < x < xlim2, y_ /; y ≤ ylim1, z_} :→ SetPrecision[{x, y + ylim2, z}, 8],
     {x_ /; x ≤ xlim1, y_ /; y ≤ ylim1, z_} :→ SetPrecision[{x + xlim2, y + ylim2, z}, 8],
     {x_ /; x ≤ xlim1, y_ /; ylim1 < y < ylim2, z_} :→ SetPrecision[{x + xlim2, y, z}, 8],
     {x_ /; x ≤ xlim1, y_ /; y ≥ ylim2, z_} :→ SetPrecision[{x + xlim2, y - ylim2, z}, 8],
     {x_ /; xlim1 < x < xlim2, y_ /; y ≥ ylim2, z_} :→ SetPrecision[{x, y - ylim2, z}, 8],
     {x_ /; x ≥ xlim2, y_ /; y ≥ ylim2, z_} :→ SetPrecision[{x - xlim2, y - ylim2, z}, 8]
    }];

  transformRules = Dispatch[{
     {x_ /; x ≥ xlim2, y_ /; y ≤ ylim1, _} :→ SetPrecision[{-xlim2, ylim2, 0}, 8],
     {x_ /; x ≥ xlim2, y_ /; ylim1 < y < ylim2, _} :→ SetPrecision[{-xlim2, 0, 0}, 8],
     {x_ /; xlim1 < x < xlim2, y_ /; y ≤ ylim1, _} :→ SetPrecision[{0, ylim2, 0}, 8],
     {x_ /; x ≤ xlim1, y_ /; y ≤ ylim1, _} :→ SetPrecision[{xlim2, ylim2, 0}, 8],
     {x_ /; x ≤ xlim1, y_ /; ylim1 < y < ylim2, _} :→ SetPrecision[{xlim2, 0, 0}, 8],
     {x_ /; x ≤ xlim1, y_ /; y ≥ ylim2, _} :→ SetPrecision[{xlim2, -ylim2, 0}, 8],
     {x_ /; xlim1 < x < xlim2, y_ /; y ≥ ylim2, _} :→ SetPrecision[{0, -ylim2, 0}, 8],
     {x_ /; x ≥ xlim2, y_ /; y ≥ ylim2, _} :→ SetPrecision[{-xlim2, -ylim2, 0}, 8],
     {___Real} :→ SetPrecision[{0, 0, 0}, 8]}];
 ];
```

In[•]:=
```
Clear@getLocalTopology;
With[{xlim1 = xLim⟦1⟧, xlim2 = xLim⟦2⟧, ylim1 = yLim⟦1⟧, ylim2 = yLim⟦2⟧},
  getLocalTopology[ptsToIndAssoc_, indToPtsAssoc_, vertexToCell_,
     cellVertexGrouping_, wrappedMat_, faceListCoords_][vertices_] :=
   Block[{localtopology = <||>, wrappedcellList = {}, vertcellconns,
      localcellunion, v, wrappedcellpos, vertcs = vertices, rl1, rl2,
      transVector, wrappedcellCoords, wrappedcells, vertOutofBounds,
      shiftedPt, transvecList = {}, $faceListCoords = Values@faceListCoords,
      vertexQ, boundsCheck, rules, extractcellkeys, vertind,
```

```
      cellsconnected, wrappedcellsrem},

     vertexQ = MatchQ[vertices, {__?NumberQ}];
     If[vertexQ,
      (vertcellconns =
        AssociationThread[{#} , {vertexToCell[ptsToIndAssoc[#]]}] &@vertices;
       vertcs = {vertices};
       localcellunion = Flatten[Values@vertcellconns]),
      (vertcellconns = AssociationThread[# ,
           Lookup[vertexToCell, Lookup[ptsToIndAssoc, #]]] &@vertices;
       localcellunion = Union@Flatten[Values@vertcellconns])
     ];
     If[localcellunion ≠ {},
      AppendTo[localtopology,
       Thread[localcellunion →
         Map[Lookup[indToPtsAssoc, #] &, cellVertexGrouping /@ localcellunion, {2}]]]
     ];
     (* condition to be an internal edge: both vertices should have 3 neighbours *)
     (* if a vertex has 3 cells in its local neighbourhood then the entire
       network topology about the vertex is known → no wrapping required *)
     (* else we need to wrap around the vertex because other cells
       are connected to it → periodic boundary conditions *)
     With[{vert = #},
        vertind = ptsToIndAssoc[vert];
        cellsconnected = vertexToCell[vertind];
        If[Length[cellsconnected] ≠ 3,
         If[(𝒟~RegionMember~Most[vert]),
           (* vertex inside bounds of the simulation domain *)
           (*Print["vertex inside bounds"];*)
           v = vert;
           With[{x = v⟦1⟧, y = v⟦2⟧},
            boundsCheck = (x == xlim1 || x == xlim2 || y == ylim1 || y == ylim2)];
           extractcellkeys = If[boundsCheck,
             {rl1, rl2} = {SetPrecision[v, 5], SetPrecision[v /. periodicRules, 5]};
             Block[{x$},
              rules = With[{r = rl1, s = rl2},
                DeleteDuplicates[HoldPattern[Equal[x$, r]] || HoldPattern[Equal[x$, s]]]
               ]
             ];
             Position @@ With[{rule = rules},
               Hold[wrappedMat, x_ /; ReleaseHold@rule, {3}]
              ],
             With[{p = SetPrecision[v, 5]},
              Position[wrappedMat, x_ /; Equal[x, p], {3}]
             ]
            ];
           (* find cell indices that are attached to the vertex in wrappedMat *)
```

```
wrappedcellpos = DeleteDuplicatesBy[
  Cases[extractcellkeys,
   {Key[p : Except[Alternatives @@ Join[localcellunion,
          Flatten@wrappedcellList]]], y__} ⧴ {p, y}], First];
(*wrappedcellpos = wrappedcellpos/.{Alternatives@@
      Flatten[wrappedcellList],__} ⧴ Sequence[];*)
(* if a wrapped cell has not been considered earlier (i.e. is new)
 then we translate it to the position of the vertex *)
If[wrappedcellpos ≠ {},
 If[vertexQ,
  transVector = SetPrecision[(v - Extract[$faceListCoords,
         Replace[#, {p_, q__} ⧴ {Key[p], q}, {1}]]) & /@ wrappedcellpos, 8],
  (* call to function is enquiring an edge and not a vertex*)
  transVector =
   SetPrecision[(v - Extract[$faceListCoords, #]) & /@ wrappedcellpos, 8]
 ];
 wrappedcellCoords = MapThread[#1 → Map[
      Function[x, SetPrecision[x + #2, 8]], $faceListCoords[[#1]], {2}] &,
   {First /@ wrappedcellpos, transVector}];
 wrappedcells = Keys[wrappedcellCoords];
 AppendTo[wrappedcellList, Flatten@wrappedcells];
 AppendTo[transvecList, transVector];
 AppendTo[localtopology, wrappedcellCoords];
],

(* the else clause: vertex is out of bounds *)
(*Print["vertex out of bounds"];*)
vertOutofBounds = vert;
(* translate the vertex back into mesh *)
transVector = vertOutofBounds /. transformRules;
shiftedPt = SetPrecision[vertOutofBounds + transVector, 5];
(* ------------- CORE B ------------- *)
(* find which cells the
 shifted vertex is a part of in the wrapped matrix *)
wrappedcells = With[{voffbounds = SetPrecision[vertOutofBounds, 5]},
  Complement[
   Union@Cases[
      Position[wrappedMat,
       x_ /; Equal[x, shiftedPt] || Equal[x, voffbounds], {3}],
      x_Key ⧴ Sequence @@ x, {2}] /. Alternatives @@
      localcellunion → Sequence[],
   Flatten@wrappedcellList]
 ];
(*forming local topology now that we know the wrapped cells *)
If[wrappedcells ≠ {},
 AppendTo[wrappedcellList, Flatten@wrappedcells];
 wrappedcellCoords = AssociationThread[wrappedcells,
```

```
      Map[Lookup[indToPtsAssoc, #] &,
        cellVertexGrouping[#] & /@ wrappedcells, {2}]];
    With[{opt = (vertOutofBounds /. periodicRules) | vertOutofBounds},
     Block[{pos, vertref, transvec},
       Do[
        With[{cellcoords = wrappedcellCoords[cell]},
         pos = FirstPosition[cellcoords /. periodicRules, opt];
         If[Head[pos] === Missing,
          Print[pos];
          pos = FirstPosition[SetPrecision[
              cellcoords /. periodicRules, 5], SetPrecision[opt, 5]];
         ];
         vertref = Extract[cellcoords, pos];
         transvec = SetPrecision[vertOutofBounds - vertref, 8];
         AppendTo[transvecList, transvec];
         AppendTo[localtopology,
          cell → Map[SetPrecision[# + transvec, 8] &, cellcoords, {2}]];
        ], {cell, wrappedcells}]
      ];
    ];
   ];
   (* to detect wrapped cells not detected by CORE B*)
   (* ------------- CORE C ------------- *)
   Block[{pos, celllocs, ls, transvec, assoc, tvecLs = {}, ckey},
    ls = Union@Flatten@Join[cellsconnected, wrappedcells];
    If[Length[ls] ≠ 3,
     pos = Position[faceListCoords, x_ /; Equal[x, shiftedPt], {3}];
     celllocs = DeleteDuplicatesBy[Cases[pos, Except[{Key[Alternatives @@ ls],
           __}]], First] /. {Key[x_], z__} :→ {Key[x], {z}};
     If[celllocs ≠ {},
      celllocs = Transpose@celllocs;
      assoc = <|
        MapThread[
         (transvec = SetPrecision[
              vertOutofBounds - Extract[faceListCoords[Sequence @@ #1], #2], 8];
          ckey = Identity @@ #1;
          AppendTo[tvecLs, transvec];
          ckey → Map[SetPrecision[Lookup[indToPtsAssoc, #] + transvec, 8] &,
            cellVertexGrouping[Sequence @@ #1], {2}]
         ) &, celllocs]
        |>;
      AppendTo[localtopology, assoc];
      AppendTo[wrappedcellList, Keys@assoc];
      AppendTo[transvecList, tvecLs];
     ];
    ];
   ];
```

```
          ];
        ];
      ] & /@ vertcs;

    transvecList = Which[
      MatchQ[transvecList, {{{__?NumberQ}}}], First[transvecList],
      MatchQ[transvecList, {{__?NumberQ} ..}], transvecList,
      True, transvecList //. {x___, {p : {__?NumberQ} ..}, y___} :> {x, p, y}
     ];
    {localtopology, Flatten@wrappedcellList, transvecList}
   ]
  ];
```

In[ ]:=

```
Clear@outerCellsFn;
outerCellsFn::Information = "the function finds the cells at the boundary";
With[{xlim1 = xLim[[1]], xlim2 = xLim[[2]], ylim1 = yLim[[1]], ylim2 = yLim[[2]]},
  outerCellsFn[faceListCoords_, vertexToCell_, ptsToIndAssoc_] :=
   Block[{res, missing, nearestpt, ptc, p1, p2, p3, boole, picks},
    ptc = Keys[ptsToIndAssoc];
    {p1, p2, p3} = Transpose@ptc;
    boole = Unitize[Boole[Thread[p1 ≤ xlim1]] + Boole[Thread[p1 ≥ xlim2]] +
       Boole[Thread[p2 ≤ ylim1]] + Boole[Thread[p2 ≥ ylim2]]];
    picks = Pick[ptc, boole, 1];
    res = Union@Flatten@Lookup[vertexToCell,
        Lookup[ptsToIndAssoc, picks~Join~(picks /. periodicRules)]
       ];
    If[MemberQ[res, _Missing, {1}],
     missing = Cases[res, Missing[_, Missing[_, y_]] :> y, {1}];
     nearestpt = Lookup[ptsToIndAssoc,
       Function[p, SelectFirst[ptc, Chop[# - p, 10^-5] == {0, 0, 0} &]] /@ missing];
     res = Union[DeleteMissing[res]~Join~Flatten@Lookup[vertexToCell, nearestpt]]
    ];
    res
   ]
  ];
```

face triangulation and associated f(x)’s

In[ ]:=
```
Clear[triangulateFaces];
triangulateFaces::Information =
  "the function takes in cell faces and triangulates them";
triangulateFaces[faces_] := Block[{edgelen, ls, mean},
   (If[Length[#] ≠ 3,
       ls = Partition[#, 2, 1, 1];
       edgelen = Norm[SetPrecision[First[#] - Last[#], 8]] & /@ ls;
       mean = Total[edgelen * (Midpoint /@ ls)] / Total[edgelen];
       mean = mean ~ SetPrecision ~ 8;
       Map[Append[#, mean] &, ls],
       {#}
      ]) & /@ faces
  ];
```

In[ ]:=
```
(*Clear[listableMeanFaces];
listableMeanFaces=Compile[{{faces,_Real,2}},
  Block[{facepart,edgelen},
   facepart=Partition[faces,2,1];
   AppendTo[facepart,{facepart[[-1,-1]],faces[[1]]}];
   edgelen=Table[Norm[Chop[First[i]-Last[i],10^-5]],{i,facepart}];
   Total[edgelen*(Mean/@facepart)]/Total[edgelen]
  ],CompilationTarget→"C",RuntimeOptions→"Speed",RuntimeAttributes→{Listable},
  CompilationOptions→{"InlineExternalDefinitions" → True}
 ]*)
```

In[ ]:=
```
ClearAll[meanFaces];
meanFaces = Compile[{{faces, _Real, 2}},
  Block[{facepart, edgelen},
   facepart = Partition[faces, 2, 1];
   AppendTo[facepart, {facepart[[-1, -1]], faces[[1]]}];
   edgelen = Table[Norm[Chop[First[i] - Last[i], 10^-5]], {i, facepart}];
   Total[edgelen * (Mean /@ facepart)] / Total[edgelen]
  ], CompilationTarget → "C", RuntimeOptions → "Speed",
  CompilationOptions → {"InlineExternalDefinitions" → True}
 ]
```

Out[ ]=
```
CompiledFunction[ Argument count: 1
                  Argument types: {{_Real, 2}} ]
```

In[ ]:=
```
CompilePrint[meanFaces]
```

Out[ ]=
```
        1 argument
```

```
        12 Integer registers
        3 Real registers
        10 Tensor registers
        Underflow checking off
        Overflow checking off
        Integer overflow checking off
        RuntimeAttributes -> {}

        T(R2)0 = A1
        I7 = 0
        I4 = 10
        I5 = 5
        I0 = 2
        I2 = -1
        I1 = 1
        Result = T(R1)7

1    T(I1)5 = {I0}
2    T(I1)3 = {I1}
3    T(R3)2 = Partition[ T(R2)0, T(I1)5, T(I1)3]]
4    T(R1)5 = Part[ T(R3)2, I2, I2]
5    T(R1)3 = Part[ T(R2)0, I1]
6    T(R2)8 = {T(R1)5, T(R1)3}
7    T(I1)5 = {I2}
8    T(I2)3 = {T(I1)5}
9    T(R3)1 = Insert[ T(R3)2, T(R2)8, T(I2)3]]
10    T(R3)2 = CopyTensor[ T(R3)1]]
11    I9 = Length[ T(R3)2]
12    I6 = I7
13    T(R1)1 = Table[ I9]
14    I3 = I7
15    goto 27
16    T(R2)3 = GetElement[ T(R3)2, I3]
17    T(R1)7 = Part[ T(R2)3, I1]
18    T(R1)8 = Part[ T(R2)3, I2]
19    T(R1)4 = - T(R1)8
20    T(R1)7 = T(R1)7 + T(R1)4
21    I10 = Power[ I4, I5]
22    R2 = I10
23    R0 = Reciprocal[ R2]
24    T(R1)4 = Chop[ T(R1)7, R0]
25    R0 = Norm[ T(R1)4, I0, I7]]
26    Element[ T(R1)1, I6] = R0
27    if[ ++ I3 <= I9] goto 16
28    I3 = Length[ T(R3)2]
29    I8 = I2
30    T(R2)3 = Table[ I3, I8]
```

```
31    I10 = I7
32    goto 40
33    T(R2)4 = GetElement[ T(R3)2, I10]
34    T(R1)8 = Total[ T(R2)4, I7]]
35    I11 = Length[ T(R2)4]
36    R0 = I11
37    R1 = Reciprocal[ R0]
38    T(R1)9 = R1 * T(R1)8
39    Element[ T(R2)3, I8] = T(R1)9
40    if[ ++ I10 <= I3] goto 33
41    T(R2)7 = T(R1)1 * T(R2)3
42    T(R1)3 = Total[ T(R2)7, I7]]
43    R1 = TotalAll[ T(R1)1, I7]]
44    R0 = Reciprocal[ R1]
45    T(R1)7 = R0 * T(R1)3
46    Return
```

In[ ]:=

```
ClearAll[triangulateToMesh];
triangulateToMesh::Information =
  "the function takes in cell faces and triangulates them";
triangulateToMesh[faces_] := Block[{mf, partfaces},
   (*mf=SetPrecision[listableMeanFaces@faces,8];*)
   mf = SetPrecision[meanFaces /@ faces, 8];
   partfaces = Partition[#, 2, 1, 1] & /@ faces;
   MapThread[
    If[Length[#] ≠ 3,
      Function[x, Join[x, {#2}]] /@ #1,
      {#[[All, 1]]}
     ] &, {partfaces, mf}]
  ];
```

In[ ]:=
```
ClearAll[tToMesh];
With[{meanFaces = meanFaces},
 tToMesh = Compile[{{face, _Real, 2}},
   Block[{mf, partface, $face = face},
    If[Length[$face] ≠ 3,
     mf = meanFaces@$face;
     partface = Partition[$face, 2, 1];
     AppendTo[partface, {Last@$face, First@$face}];
     Map[Join[#, {mf}] &, partface],
     {$face}
    ]
   ],
   CompilationTarget → "C", RuntimeOptions → "Speed", CompilationOptions →
    {"InlineCompiledFunctions" → True, "ExpressionOptimization" → False}
  ]
]
```

Out[ ]= CompiledFunction[Argument count: 1 Argument types: {{_Real, 2}}]

In[ ]:=
```
CompilePrint[tToMesh]
```

Out[ ]=
```
        1 argument
        1 Boolean register
        13 Integer registers
        3 Real registers
        13 Tensor registers
        Underflow checking off
        Overflow checking off
        Integer overflow checking off
        RuntimeAttributes -> {}

        T(R2)0 = A1
        I8 = 0
        I5 = 10
        I6 = 5
        I2 = 2
        I4 = -1
        I3 = 1
        I1 = 3
        Result = T(R3)12

1    T(R2)1 = CopyTensor[ T(R2)0]]
2    I9 = Length[ T(R2)1]
3    B0 = I9 == I1
4    B0 = ! B0
```

```
5    if[ !B0] goto 74
6    T(R2)3 = CopyTensor[ T(R2)1]]
7    T(I1)8 = {I2}
8    T(I1)2 = {I3}
9    T(R3)5 = Partition[ T(R2)3, T(I1)8, T(I1)2]]
10    T(R1)8 = Part[ T(R3)5, I4, I4]
11    T(R1)2 = Part[ T(R2)3, I3]
12    T(R2)10 = {T(R1)8, T(R1)2}
13    T(I1)8 = {I4}
14    T(I2)2 = {T(I1)8}
15    T(R3)9 = Insert[ T(R3)5, T(R2)10, T(I2)2]]
16    T(R3)5 = CopyTensor[ T(R3)9]]
17    I0 = Length[ T(R3)5]
18    I11 = I8
19    T(R1)9 = Table[ I0]
20    I9 = I8
21    goto 33
22    T(R2)2 = GetElement[ T(R3)5, I9]
23    T(R1)6 = Part[ T(R2)2, I3]
24    T(R1)10 = Part[ T(R2)2, I4]
25    T(R1)4 = - T(R1)10
26    T(R1)6 = T(R1)6 + T(R1)4
27    I10 = Power[ I5, I6]
28    R2 = I10
29    R0 = Reciprocal[ R2]
30    T(R1)4 = Chop[ T(R1)6, R0]
31    R0 = Norm[ T(R1)4, I2, I8]]
32    Element[ T(R1)9, I11] = R0
33    if[ ++ I9 <= I0] goto 22
34    I9 = Length[ T(R3)5]
35    I7 = I4
36    T(R2)2 = Table[ I9, I7]
37    I10 = I8
38    goto 46
39    T(R2)4 = GetElement[ T(R3)5, I10]
40    T(R1)10 = Total[ T(R2)4, I8]]
41    I12 = Length[ T(R2)4]
42    R0 = I12
43    R1 = Reciprocal[ R0]
44    T(R1)12 = R1 * T(R1)10
45    Element[ T(R2)2, I7] = T(R1)12
46    if[ ++ I10 <= I9] goto 39
47    T(R2)6 = T(R1)9 * T(R2)2
48    T(R1)2 = Total[ T(R2)6, I8]]
49    R1 = TotalAll[ T(R1)9, I8]]
50    R0 = Reciprocal[ R1]
51    T(R1)6 = R0 * T(R1)2
```

```
52    T(I1)3 = {I2}
53    T(I1)7 = {I3}
54    T(R3)9 = Partition[ T(R2)1, T(I1)3, T(I1)7]]
55    T(R1)3 = Part[ T(R2)1, I4]
56    T(R1)7 = Part[ T(R2)1, I3]
57    T(R2)5 = {T(R1)3, T(R1)7}
58    T(I1)3 = {I4}
59    T(I2)7 = {T(I1)3}
60    T(R3)2 = Insert[ T(R3)9, T(R2)5, T(I2)7]]
61    T(R3)9 = CopyTensor[ T(R3)2]]
62    I0 = Length[ T(R3)9]
63    I9 = I4
64    T(R3)2 = Table[ I0, I3, I9]
65    I7 = I8
66    goto 71
67    T(R2)5 = GetElement[ T(R3)9, I7]
68    T(R2)7 = {T(R1)6}
69    T(R2)12 = Join[ T(R2)5, T(R2)7]]
70    Element[ T(R3)2, I9] = T(R2)12
71    if[ ++ I7 <= I0] goto 67
72    T(R3)12 = CopyTensor[ T(R3)2]]
73    goto 76
74    T(R3)3 = {T(R2)1}
75    T(R3)12 = CopyTensor[ T(R3)3]]
76    Return
```

In[ ]:=
```
ClearAll[localTriFunc];
With[{meanFaces = meanFaces},
 localTriFunc = Compile[{{ls, _Real, 2}, {pt, _Real, 1}},
   Block[{$face, k = 0, unit, len, mf, u},
    $face = ls;
    unit = Chop[Transpose[Transpose[$face] - pt], 10^-5];
    len = Length[unit];
    Do[
     If[unit[[i]] == {0, 0, 0},
      k = i;
      Break[];
     ], {i, len}
    ];
    If[k ≠ 0,
     If[len == 3,
      $face,
      mf = meanFaces@$face;
      Which[
       k == 1,
       u = Compile`GetElement[$face, 1];
       {Compile`GetElement[$face, len], u, mf, u, Compile`GetElement[$face, 2], mf},
       k == len,
       u = Compile`GetElement[$face, len];
       {Compile`GetElement[$face, len - 1], u, mf, u, Compile`GetElement[$face, 1], mf},
       True,
       u = Compile`GetElement[$face, k];
       {Compile`GetElement[$face, k - 1], u, mf, u, Compile`GetElement[$face, k + 1], mf}
      ]
     ],
     {{0}}
    ]
   ], CompilationTarget → "C", RuntimeOptions → "Speed",
   RuntimeAttributes → {Listable}, Parallelization → True,
   CompilationOptions → {"InlineCompiledFunctions" → True}
  ]
]
```

Out[ ]= CompiledFunction[Argument count: 2
Argument types: {{_Real, 2}, {_Real, 1}}]

In[ ]:= `CompilePrint[localTriFunc]`

Out[ ]=

```
2 arguments
4 Boolean registers
16 Integer registers
4 Real registers
```

```
        16 Tensor registers
        Underflow checking off
        Overflow checking off
        Integer overflow checking off
        RuntimeAttributes -> {Listable}

        T(R2)0 = A1
        T(R1)1 = A2
        I0 = 0
        I1 = 10
        I2 = 5
        T(I1)6 = {0, 0, 0}
        T(I2)15 = {{0}}
        I9 = 2
        I11 = -1
        I10 = 1
        I8 = 3
        R2 = 0.
        Result = T(R2)11

1    I3 = I0
2    T(R2)5 = CopyTensor[ T(R2)0]]
3    T(R2)2 = Transpose[ T(R2)5]]
4    T(R1)3 = - T(R1)1
5    T(R2)4 = T(R2)2 + T(R1)3
6    T(R2)2 = Transpose[ T(R2)4]]
7    I4 = Power[ I1, I2]
8    R0 = I4
9    R1 = Reciprocal[ R0]
10    T(R2)4 = Chop[ T(R2)2, R1]
11    I4 = Length[ T(R2)4]
12    I6 = I4
13    I7 = I0
14    goto 21
15    T(R1)2 = Part[ T(R2)4, I7]
16    B0 = CompareTensor[ I2, R2, T(R1)2, T(I1)6]]
17    if[ !B0] goto 21
18    I3 = I7
19    goto 22
20    goto 21
21    if[ ++ I7 <= I6] goto 15
22    B0 = I3 == I0
23    B0 = ! B0
24    if[ !B0] goto 105
25    B1 = I4 == I8
26    if[ !B1] goto 29
27    T(R2)7 = CopyTensor[ T(R2)5]]
```

```
28    goto 103
29    T(R2)2 = CopyTensor[ T(R2)5]]
30    T(I1)10 = {I9}
31    T(I1)8 = {I10}
32    T(R3)7 = Partition[ T(R2)2, T(I1)10, T(I1)8]]
33    T(R1)10 = Part[ T(R3)7, I11, I11]
34    T(R1)8 = Part[ T(R2)2, I10]
35    T(R2)13 = {T(R1)10, T(R1)8}
36    T(I1)10 = {I11}
37    T(I2)8 = {T(I1)10}
38    T(R3)3 = Insert[ T(R3)7, T(R2)13, T(I2)8]]
39    T(R3)7 = CopyTensor[ T(R3)3]]
40    I13 = Length[ T(R3)7]
41    I7 = I0
42    T(R1)3 = Table[ I13]
43    I6 = I0
44    goto 56
45    T(R2)8 = GetElement[ T(R3)7, I6]
46    T(R1)12 = Part[ T(R2)8, I10]
47    T(R1)13 = Part[ T(R2)8, I11]
48    T(R1)9 = - T(R1)13
49    T(R1)12 = T(R1)12 + T(R1)9
50    I14 = Power[ I1, I2]
51    R3 = I14
52    R1 = Reciprocal[ R3]
53    T(R1)9 = Chop[ T(R1)12, R1]
54    R1 = Norm[ T(R1)9, I9, I0]]
55    Element[ T(R1)3, I7] = R1
56    if[ ++ I6 <= I13] goto 45
57    I6 = Length[ T(R3)7]
58    I12 = I11
59    T(R2)8 = Table[ I6, I12]
60    I14 = I0
61    goto 69
62    T(R2)9 = GetElement[ T(R3)7, I14]
63    T(R1)13 = Total[ T(R2)9, I0]]
64    I15 = Length[ T(R2)9]
65    R1 = I15
66    R0 = Reciprocal[ R1]
67    T(R1)14 = R0 * T(R1)13
68    Element[ T(R2)8, I12] = T(R1)14
69    if[ ++ I14 <= I6] goto 62
70    T(R2)12 = T(R1)3 * T(R2)8
71    T(R1)8 = Total[ T(R2)12, I0]]
72    R0 = TotalAll[ T(R1)3, I0]]
73    R1 = Reciprocal[ R0]
74    T(R1)12 = R1 * T(R1)8
```

```
75    B2 = I3 == I10
76    if[ !B2] goto 83
77    T(R1)2 = GetElement[ T(R2)5, I10]
78    T(R1)11 = GetElement[ T(R2)5, I4]
79    T(R1)3 = GetElement[ T(R2)5, I9]
80    T(R2)7 = {T(R1)11, T(R1)2, T(R1)12, T(R1)2, T(R1)3, T(R1)12}
81    T(R2)8 = CopyTensor[ T(R2)7]]
82    goto 102
83    B3 = I3 == I4
84    if[ !B3] goto 93
85    T(R1)11 = GetElement[ T(R2)5, I4]
86    T(R1)2 = CopyTensor[ T(R1)11]]
87    I14 = I4 + I11
88    T(R1)11 = GetElement[ T(R2)5, I14]
89    T(R1)3 = GetElement[ T(R2)5, I10]
90    T(R2)8 = {T(R1)11, T(R1)2, T(R1)12, T(R1)2, T(R1)3, T(R1)12}
91    T(R2)11 = CopyTensor[ T(R2)8]]
92    goto 101
93    T(R1)11 = GetElement[ T(R2)5, I3]
94    T(R1)2 = CopyTensor[ T(R1)11]]
95    I14 = I3 + I11
96    T(R1)11 = GetElement[ T(R2)5, I14]
97    I14 = I3 + I10
98    T(R1)3 = GetElement[ T(R2)5, I14]
99    T(R2)14 = {T(R1)11, T(R1)2, T(R1)12, T(R1)2, T(R1)3, T(R1)12}
100    T(R2)11 = CopyTensor[ T(R2)14]]
101    T(R2)8 = CopyTensor[ T(R2)11]]
102    T(R2)7 = CopyTensor[ T(R2)8]]
103    T(R2)11 = CopyTensor[ T(R2)7]]
104    goto 107
105    T(R2)14 = CoerceTensor[ I8, T(I2)15]]
106    T(R2)11 = CopyTensor[ T(R2)14]]
107    Return
```

In[ ]:=
```
Clear[areaTriFn];
areaTriFn::Information = "areaTriFn finds the area of a triangle";
areaTriFn = Compile[{{face, _Real, 2}},
  Block[{v1, v2, f = face, firstelem, v1x, v1y, v1z, v2x, v2y, v2z, cross, vx, vy, vz},
   firstelem = Compile`GetElement[f, 1];
   v2 = Compile`GetElement[f, 2] - firstelem;
   v1 = Compile`GetElement[f, 3] - firstelem;
   {v1x, v1y, v1z} = v1;
   {v2x, v2y, v2z} = v2;
   (*0.5Norm[Cross[v2,v1]]*)
   {vx, vy, vz} = {v1z v2y - v1y v2z, -v1z v2x + v1x v2z, v1y v2x - v1x v2y};
   0.5 Sqrt[vx * vx + vy * vy + vz * vz]
  ], CompilationTarget → "C", RuntimeOptions → "Speed"
 ]
```

Out[ ]= CompiledFunction[Argument count: 1
Argument types: {{_Real, 2}}]

In[ ]:= CompilePrint[areaTriFn]

Out[ ]=
```
        1 argument
        1 Boolean register
        4 Integer registers
        13 Real registers
        6 Tensor registers
        Underflow checking off
        Overflow checking off
        Integer overflow checking off
        RuntimeAttributes -> {}

        T(R2)0 = A1
        I1 = 2
        I0 = 1
        I2 = 3
        R11 = 0.5
        Result = R9

1    T(R2)1 = CopyTensor[ T(R2)0]]
2    T(R1)2 = GetElement[ T(R2)1, I0]
3    T(R1)3 = GetElement[ T(R2)1, I1]
4    T(R1)4 = - T(R1)2
5    T(R1)3 = T(R1)3 + T(R1)4
6    T(R1)4 = GetElement[ T(R2)1, I2]
7    T(R1)5 = - T(R1)2
8    T(R1)4 = T(R1)4 + T(R1)5
9    T(R1)5 = CopyTensor[ T(R1)4]]
```

```
10    I3 = Length[ T(R1)5]
11    B0 = I3 == I2
12    B0 = ! B0
13    if[ !B0] goto 16
14    Return Error
15    goto 16
16    R0 = GetElement[ T(R1)5, I0]
17    R1 = GetElement[ T(R1)5, I1]
18    R2 = GetElement[ T(R1)5, I2]
19    T(R1)5 = CopyTensor[ T(R1)3]]
20    I3 = Length[ T(R1)5]
21    B0 = I3 == I2
22    B0 = ! B0
23    if[ !B0] goto 26
24    Return Error
25    goto 26
26    R3 = GetElement[ T(R1)5, I0]
27    R4 = GetElement[ T(R1)5, I1]
28    R5 = GetElement[ T(R1)5, I2]
29    R6 = R2 * R4
30    R7 = R1 * R5
31    R8 = - R7
32    R6 = R6 + R8
33    R8 = - R2
34    R8 = R8 * R3
35    R7 = R0 * R5
36    R8 = R8 + R7
37    R7 = R1 * R3
38    R9 = R0 * R4
39    R10 = - R9
40    R7 = R7 + R10
41    T(R1)5 = {R6, R8, R7}
42    I3 = Length[ T(R1)5]
43    B0 = I3 == I2
44    B0 = ! B0
45    if[ !B0] goto 48
46    Return Error
47    goto 48
48    R6 = GetElement[ T(R1)5, I0]
49    R8 = GetElement[ T(R1)5, I1]
50    R7 = GetElement[ T(R1)5, I2]
51    R9 = R6 * R6
52    R10 = R8 * R8
53    R12 = R7 * R7
54    R9 = R9 + R10 + R12
55    R10 = Sqrt[ R9]
56    R9 = R11 * R10
```

```
57    Return
```

```
(*ClearAll[meanTri];
meanTri::Information="meanTri returns the centroid of the triangle";
meanTri=Compile[{{faces,_Real,2}},
  Mean@faces,
  CompilationTarget→"C",RuntimeAttributes→{Listable},RuntimeOptions→"Speed"
 ]*)
```

```
(*ClearAll[meanTri];
meanTri::Information="meanTri returns the centroid of the triangle";
meanTri=Compile[{{faces,_Real,2}},
  Block[{vec},
   vec=faces;
   (Compile`GetElement[vec,1]+
      Compile`GetElement[vec,2]+Compile`GetElement[vec,3])/3.0
  ],
  CompilationTarget→"C",RuntimeAttributes→{Listable},RuntimeOptions→"Speed"
 ]*)
```

In[ ]:=

```
ClearAll[meanTri];
meanTri::Information = "meanTri returns the centroid of the triangle";
meanTri = Compile[{{faces, _Real, 2}},
  Total[faces] / 3.0,
  CompilationTarget → "C", RuntimeAttributes → {Listable}, RuntimeOptions → "Speed"
 ]
```

Out[ ]=

```
CompiledFunction[ Argument count: 1
                  Argument types: {{_Real, 2}} ]
```

In[ ]:=
```
CompilePrint[meanTri]
```

Out[ ]=
```
        1 argument
        1 Integer register
        1 Real register
        3 Tensor registers
        Underflow checking off
        Overflow checking off
        Integer overflow checking off
        RuntimeAttributes -> {Listable}

        T(R2)0 = A1
        I0 = 0
        R0 = 0.3333333333333333
        Result = T(R1)2

1    T(R1)1 = Total[ T(R2)0, I0]]
2    T(R1)2 = R0 * T(R1)1
3    Return
```

```
(*Clear[triNormal];
triNormal::Information="triNormal returns the normal of a triangle face";
triNormal=Compile[{{ls,_Real,2}},
  Block[{res},
   res=Partition[ls,2,1];
   Cross[res[[1,1]]-res[[1,2]],res[[2,1]]-res[[2,2]]]
  ],CompilationTarget→"C",RuntimeAttributes→{Listable},
  RuntimeOptions→"Speed"
 ]*)
```

In[ ]:=
```
ClearAll[triNormal];
triNormal::Information = "triNormal returns the normal of a triangle face";
triNormal = Compile[{{ls, _Real, 2}},
  Block[{vecs = ls, p1, v, w, vx, vy, vz, wx, wy, wz},
   p1 = Compile`GetElement[vecs, 1];
   v = Compile`GetElement[vecs, 2] - p1;
   w = Compile`GetElement[vecs, 3] - p1;
   vx = Compile`GetElement[v, 1];
   vy = Compile`GetElement[v, 2];
   vz = Compile`GetElement[v, 3];
   wx = Compile`GetElement[w, 1];
   wy = Compile`GetElement[w, 2];
   wz = Compile`GetElement[w, 3];
   {vy wz - vz wy, vz wx - vx wz, vx wy - vy wx}
  ], CompilationTarget → "C", RuntimeOptions → "Speed"
 ]
```

Out[ ]= CompiledFunction[Argument count: 1 Argument types: {{_Real, 2}}]

```
In[∘]:= CompilePrint[triNormal]

Out[∘]=
        1 argument
        3 Integer registers
        11 Real registers
        6 Tensor registers
        Underflow checking off
        Overflow checking off
        Integer overflow checking off
        RuntimeAttributes -> {}

        T(R2)0 = A1
        I1 = 2
        I0 = 1
        I2 = 3
        Result = T(R1)5

1    T(R2)1 = CopyTensor[ T(R2)0]]
2    T(R1)2 = GetElement[ T(R2)1, I0]
3    T(R1)3 = GetElement[ T(R2)1, I1]
4    T(R1)4 = - T(R1)2
5    T(R1)3 = T(R1)3 + T(R1)4
6    T(R1)4 = GetElement[ T(R2)1, I2]
7    T(R1)5 = - T(R1)2
8    T(R1)4 = T(R1)4 + T(R1)5
9    R0 = GetElement[ T(R1)3, I0]
10    R1 = GetElement[ T(R1)3, I1]
11    R2 = GetElement[ T(R1)3, I2]
12    R3 = GetElement[ T(R1)4, I0]
13    R4 = GetElement[ T(R1)4, I1]
14    R5 = GetElement[ T(R1)4, I2]
15    R6 = R1 * R5
16    R7 = R2 * R4
17    R8 = - R7
18    R6 = R6 + R8
19    R8 = R2 * R3
20    R7 = R0 * R5
21    R9 = - R7
22    R8 = R8 + R9
23    R9 = R0 * R4
24    R7 = R1 * R3
25    R10 = - R7
26    R9 = R9 + R10
27    T(R1)5 = {R6, R8, R9}
28    Return
```

In[*]:=
```
ClearAll[normNormal];
normNormal::Information =
  "normNormal returns the normalized normal of a triangle face";
normNormal = Compile[{{ls, _Real, 1}},
  Block[{vecs = ls, x, y, z},
   x = Compile`GetElement[vecs, 1];
   y = Compile`GetElement[vecs, 2];
   z = Compile`GetElement[vecs, 3];
   {x, y, z} / Sqrt[(x x) + (y y) + (z z)]
  ], CompilationTarget → "C", RuntimeOptions → "Speed"
 ]
```

Out[*]=
```
CompiledFunction[ Argument count: 1
                  Argument types: {{_Real, 1}} ]
```

In[∘]:=
```
CompilePrint[normNormal]
```

Out[∘]=
```
        1 argument
        3 Integer registers
        6 Real registers
        4 Tensor registers
        Underflow checking off
        Overflow checking off
        Integer overflow checking off
        RuntimeAttributes -> {}

        T(R1)0 = A1
        I1 = 2
        I0 = 1
        I2 = 3
        Result = T(R1)3

1    T(R1)1 = CopyTensor[ T(R1)0]]
2    R0 = GetElement[ T(R1)1, I0]
3    R1 = GetElement[ T(R1)1, I1]
4    R2 = GetElement[ T(R1)1, I2]
5    T(R1)2 = {R0, R1, R2}
6    R3 = R0 * R0
7    R4 = R1 * R1
8    R5 = R2 * R2
9    R3 = R3 + R4 + R5
10    R4 = Sqrt[ R3]
11    R3 = Reciprocal[ R4]
12    T(R1)3 = R3 * T(R1)2
13    Return
```

In[∘]:=
```
Clear[lenEdge];
lenEdge::Information = "lenEdge returns the length of an edge";
lenEdge = Compile[{{edge1, _Real, 1}, {edge2, _Real, 1}},
  Norm[Chop[edge1 - edge2, 10^-5]],
  CompilationTarget → "C", CompilationOptions → {"InlineExternalDefinitions" → True},
  RuntimeOptions → "Speed"
 ]
```

Out[∘]=
```
CompiledFunction[ Argument count: 2
                  Argument types: {{_Real, 1}, {_Real, 1}} ]
```

In[ ]:=
```
CompilePrint[lenEdge]
```

Out[ ]=
```
        2 arguments
        5 Integer registers
        2 Real registers
        5 Tensor registers
        Underflow checking off
        Overflow checking off
        Integer overflow checking off
        RuntimeAttributes -> {}

        T(R1)0 = A1
        T(R1)1 = A2
        I4 = 0
        I0 = 10
        I1 = 5
        I3 = 2
        Result = R0

1   T(R1)3 = - T(R1)1
2   T(R1)4 = T(R1)0 + T(R1)3
3   I2 = Power[ I0, I1]
4   R1 = I2
5   R0 = Reciprocal[ R1]
6   T(R1)3 = Chop[ T(R1)4, R0]
7   R0 = Norm[ T(R1)3, I3, I4]]
8   Return
```

centroid/volume for polyhedral cells

In[ ]:=
```
(*Clear@volumePolyhedra;
volumePolyhedra::Information =
 "returns the volume of the triangulated polyhedral cell";
volumePolyhedra[facecollec_]:=1./6Total[Flatten@volumePolyhedHelper[facecollec]];

Clear@volumePolyhedHelper;
volumePolyhedHelper=Compile[{{triFaces,_Real,2}},
  Block[{V1,V2,V3},
   {V1,V2,V3}=triFaces;
   Cross[V1,V2].V3
  ],CompilationTarget→"C",RuntimeAttributes→{Listable},
  RuntimeOptions→"Speed"
 ];
```

```
*)

(*ClearAll@volumePolyhedra;
volumePolyhedra::Information =
 "returns the volume of the triangulated polyhedral cell";
volumePolyhedra[facecollec_]:=1./6Total[Flatten@volumePolyhedHelper[facecollec]];

ClearAll@volumePolyhedHelper;
volumePolyhedHelper=Compile[{{triFaces,_Real,2}},
  Block[{V1,V2,V3,v1x,v1y,v1z,v2x,v2y,v2z},
   {V1,V2,V3}=triFaces;
   {v1x,v1y,v1z}=V1;
   {v2x,v2y,v2z}=V2;
   (-v1z v2y + v1y v2z)Compile`GetElement[V3,1]+(v1z v2x -v1x v2z)
     Compile`GetElement[V3,2]+(-v1y v2x + v1x v2y)Compile`GetElement[V3,3]
  ],CompilationTarget→"C",RuntimeAttributes→{Listable},
  RuntimeOptions→"Speed"
 ];
*)

ClearAll[volumePolyhedra];
volumePolyhedra::Information =
  "returns the volume of the triangulated polyhedral cell";
volumePolyhedra[facecollec_] :=
  1. / 6 Total[Flatten[Map[volumePolyhedHelper, facecollec, {2}]]];

ClearAll@volumePolyhedHelper;
volumePolyhedHelper = Compile[{{triFaces, _Real, 2}},
   Block[{V1, V2, V3, v1x, v1y, v1z, v2x, v2y, v2z},
    {V1, V2, V3} = triFaces;
    {v1x, v1y, v1z} = V1;
    {v2x, v2y, v2z} = V2;
    (-v1z v2y + v1y v2z) Compile`GetElement[V3, 1] + (v1z v2x - v1x v2z)
      Compile`GetElement[V3, 2] + (-v1y v2x + v1x v2y) Compile`GetElement[V3, 3]
   ], CompilationTarget → "C", RuntimeOptions → "Speed"
  ];
```

In[•]:=
```
CompilePrint[volumePolyhedHelper]
```

Out[•]=
```
1 argument
1 Boolean register
4 Integer registers
10 Real registers
5 Tensor registers
Underflow checking off
Overflow checking off
Integer overflow checking off
```

```
RuntimeAttributes -> {}

T(R2)0 = A1
I3 = 2
I2 = 1
I1 = 3
Result = R6

1    T(R2)1 = CopyTensor[ T(R2)0]]
2    I0 = Length[ T(R2)1]
3    B0 = I0 == I1
4    B0 = ! B0
5    if[ !B0] goto 8
6    Return Error
7    goto 8
8    T(R1)2 = GetElement[ T(R2)1, I2]
9    T(R1)3 = GetElement[ T(R2)1, I3]
10    T(R1)4 = GetElement[ T(R2)1, I1]
11    T(R1)1 = CopyTensor[ T(R1)2]]
12    I0 = Length[ T(R1)1]
13    B0 = I0 == I1
14    B0 = ! B0
15    if[ !B0] goto 18
16    Return Error
17    goto 18
18    R0 = GetElement[ T(R1)1, I2]
19    R1 = GetElement[ T(R1)1, I3]
20    R2 = GetElement[ T(R1)1, I1]
21    T(R1)1 = CopyTensor[ T(R1)3]]
22    I0 = Length[ T(R1)1]
23    B0 = I0 == I1
24    B0 = ! B0
25    if[ !B0] goto 28
26    Return Error
27    goto 28
28    R3 = GetElement[ T(R1)1, I2]
29    R4 = GetElement[ T(R1)1, I3]
30    R5 = GetElement[ T(R1)1, I1]
31    R6 = - R2
32    R6 = R6 * R4
33    R7 = R1 * R5
34    R6 = R6 + R7
35    R7 = GetElement[ T(R1)4, I2]
36    R6 = R6 * R7
37    R7 = R2 * R3
38    R8 = R0 * R5
39    R9 = - R8
```

```
R7 = R7 + R9
R9 = GetElement[ T(R1)4, I3]
R7 = R7 * R9
R9 = - R1
R9 = R9 * R3
R8 = R0 * R4
R9 = R9 + R8
R8 = GetElement[ T(R1)4, I1]
R9 = R9 * R8
R6 = R6 + R7 + R9
Return
```

In[]:=
```
(*ClearAll@centroidPolyhedra;
centroidPolyhedra::Information =
 "returns the centroid of the triangulated polyhedral cell";
centroidPolyhedra[polyhed_,vol_]:=
 1/(2. vol)1./24Total[Flatten[centroidPolyhedraHelper@polyhed,1]];

ClearAll@centroidPolyhedraHelper;
With[{triNormal=triNormal},
 centroidPolyhedraHelper=Compile[{{triFaces,_Real,2}},
   Block[{V1,V2,V3,normal},
    {V1,V2,V3}=triFaces;
    normal=triNormal@triFaces;
    normal((V1+V2)^2 + (V2+V3)^2+(V3+V1)^2)
   ],CompilationTarget→"C",RuntimeAttributes→{Listable},
   RuntimeOptions→"Speed"
  ]
]*)

ClearAll@centroidPolyhedra;
centroidPolyhedra::Information =
  "returns the centroid of the triangulated polyhedral cell";
centroidPolyhedra[polyhed_, vol_] := 1 / (2. vol) × 1. / 24
   Total[Flatten[Map[centroidPolyhedraHelper, polyhed, {2}], 1]];

ClearAll@centroidPolyhedraHelper;
With[{triNormal = triNormal},
 centroidPolyhedraHelper = Compile[{{triFaces, _Real, 2}},
   Block[{V1, V2, V3, normal},
    {V1, V2, V3} = triFaces;
    normal = triNormal@triFaces;
    normal ((V1 + V2) ^2 + (V2 + V3) ^2 + (V3 + V1) ^2)
   ], CompilationTarget → "C", RuntimeOptions → "Speed"
  ]
]
```

Out[]= CompiledFunction[Argument count: 1 Argument types: {{_Real, 2}}]

In[ ]:= **CompilePrint[centroidPolyhedraHelper]**

Out[ ]=

```
        1 argument
        1 Boolean register
        4 Integer registers
        9 Tensor registers
        Underflow checking off
        Overflow checking off
        Integer overflow checking off
        RuntimeAttributes -> {}

        T(R2)0 = A1
        I3 = 2
        I2 = 1
        I1 = 3
        Result = T(R1)7

1    T(R2)1 = CopyTensor[ T(R2)0]]
2    I0 = Length[ T(R2)1]
3    B0 = I0 == I1
4    B0 = ! B0
5    if[ !B0] goto 8
6    Return Error
7    goto 8
8    T(R1)2 = GetElement[ T(R2)1, I2]
9    T(R1)3 = GetElement[ T(R2)1, I3]
10    T(R1)4 = GetElement[ T(R2)1, I1]
11    T(R1)1 = LibraryFunction[<>,
  compiledFunction6, {{Real, 2, Constant}}, {Real, 1}][ T(R2)0]]
12    T(R1)5 = T(R1)2 + T(R1)3
13    T(R1)6 = Square[ T(R1)5]
14    T(R1)5 = T(R1)3 + T(R1)4
15    T(R1)7 = Square[ T(R1)5]
16    T(R1)5 = T(R1)4 + T(R1)2
17    T(R1)8 = Square[ T(R1)5]
18    T(R1)6 = T(R1)6 + T(R1)7 + T(R1)8
19    T(R1)7 = T(R1)1 * T(R1)6
20    Return
```

In[ ]:=
```
Clear@parPolyhedProp;
parPolyhedProp::Information =
  "returns the centroid and volume of the polyhedral cells
    in the mesh using built-in modules";
parPolyhedProp[polyhedra_] := Module[{vals = Values@polyhedra, ls = {}, rcent, rvol},
   SetSharedVariable[ls];
   ParallelDo[AppendTo[ls, {RegionCentroid[i], Volume[i]}], {i, vals}];
   Transpose@ls
  ];
```

centroids of the local polyhedral neighbourhood

the version below uses the shift vector and is more optimized in terms of speed

In[ ]:=
```
Clear[cellCentroids];
cellCentroids::Information =
  "the function yields the centroids of the polyhedral cells
    present in the local cell topology";
cellCentroids[polyhedCentAssoc_, keystopo_, shiftvec_] :=
  Block[{assoc = <||>, regcent, counter},
   AssociationThread[Keys@keystopo →
     KeyValueMap[
      Function[{key, cellassoc},
       If[KeyFreeQ[shiftvec, key],
        Lookup[polyhedCentAssoc, cellassoc],
        If[KeyFreeQ[shiftvec[key], #],
           regcent = polyhedCentAssoc[#],
           regcent = SetPrecision[polyhedCentAssoc[#] + shiftvec[key][#], 8];
           regcent
          ] & /@ cellassoc
       ]
      ], keystopo]
   ]
  ];
```

form local topology by shifting cells

In[◦]:=
```
Clear[cellTranslator];
cellTranslator[facelsc_, keyslocaltopo_, shiftVecA_, vertkeys_] :=
  Block[{shiftvec, svkeys, cellids},
   <|Table[
     cellids = keyslocaltopo[i];
     i → If[KeyFreeQ[shiftVecA, i],
       {AssociationThread[cellids, Lookup[facelsc, cellids]], {}, {}},
       shiftvec = shiftVecA[i];
       svkeys = Keys@shiftvec;
       {AssociationThread[cellids,
         If[FreeQ[svkeys, #],
            facelsc[#],
            Map[Function[fc, SetPrecision[fc + shiftvec[#], 8]], facelsc[#], {2}]
           ] & /@ cellids], svkeys, Values@shiftvec}
      ], {i, vertkeys}]|>
  ];
```

surface ∇

In[◦]:=
```
ClearAll[rotateSourceVertOrderFn];
rotateSourceVertOrderFn = Compile[{{sourcept, _Real, 1}, {ls, _Real, 3}},
  Block[{vec, pos = 0},
   (vec = #;
      If[Chop[Compile`GetElement[vec, 1] - sourcept, 10^-8] == {0., 0., 0.},
       vec,
       Which[
        Chop[Compile`GetElement[vec, 2] - sourcept, 10^-8] == {0., 0., 0.},
        pos = 2,
        Chop[Compile`GetElement[vec, 3] - sourcept, 10^-8] == {0., 0., 0.},
        pos = 3
       ];
       RotateLeft[vec, pos - 1]
      ]) & /@ ls
  ], CompilationTarget → "C", RuntimeOptions → "Speed", CompilationOptions →
   {"ExpressionOptimization" → True, "InlineExternalDefinitions" → True}]
```

Out[◦]= CompiledFunction[Argument count: 2
Argument types: {{_Real, 1}, {_Real, 3}}]

In[◦]:=
```
CompilePrint[rotateSourceVertOrderFn]
```

Out[•]=

```
2 arguments
4 Boolean registers
15 Integer registers
3 Real registers
9 Tensor registers
Underflow checking off
Overflow checking off
Integer overflow checking off
RuntimeAttributes -> {}

T(R1)0 = A1
T(R3)1 = A2
I0 = 0
T(R1)5 = {0., 0., 0.}
I6 = 10
I7 = 8
I9 = 5
I10 = 2
I12 = -1
I4 = 1
I11 = 3
R2 = 0.
Result = T(R3)3

1    I5 = I0
2    I8 = Length[ T(R3)1]
3    I13 = I12
4    T(R3)3 = Table[ I8, I4, I13]
5    I3 = I0
6    goto 46
7    T(R2)4 = GetElement[ T(R3)1, I3]
8    T(R1)6 = GetElement[ T(R2)4, I4]
9    T(R1)8 = - T(R1)0
10    T(R1)6 = T(R1)6 + T(R1)8
11    I14 = Power[ I6, I7]
12    R0 = I14
13    R1 = Reciprocal[ R0]
14    T(R1)8 = Chop[ T(R1)6, R1]
15    B0 = CompareTensor[ I9, R2, T(R1)8, T(R1)5]]
16    if[ !B0] goto 19
17    T(R2)8 = CopyTensor[ T(R2)4]]
18    goto 45
19    T(R1)8 = GetElement[ T(R2)4, I10]
20    T(R1)6 = - T(R1)0
21    T(R1)8 = T(R1)8 + T(R1)6
22    I14 = Power[ I6, I7]
```

```
23    R1 = I14
24    R0 = Reciprocal[ R1]
25    T(R1)6 = Chop[ T(R1)8, R0]
26    B1 = CompareTensor[ I9, R2, T(R1)6, T(R1)5]]
27    if[ !B1] goto 30
28    I5 = I10
29    goto 41
30    T(R1)6 = GetElement[ T(R2)4, I11]
31    T(R1)8 = - T(R1)0
32    T(R1)6 = T(R1)6 + T(R1)8
33    I14 = Power[ I6, I7]
34    R0 = I14
35    R1 = Reciprocal[ R0]
36    T(R1)8 = Chop[ T(R1)6, R1]
37    B2 = CompareTensor[ I9, R2, T(R1)8, T(R1)5]]
38    if[ !B2] goto 41
39    I5 = I11
40    goto 41
41    I14 = I5 + I12
42    T(I1)8 = {I14}
43    T(R2)6 = RotateLeft[ T(R2)4, T(I1)8]]
44    T(R2)8 = CopyTensor[ T(R2)6]]
45    Element[ T(R3)3, I13] = T(R2)8
46    if[ ++ I3 <= I8] goto 7
47    Return
```

In[*]:=
```
ClearAll[surfaceGrad, cc, co];
surfaceGrad::Information =
  "surfaceGrad takes in arguments and computes the surface gradient about a point";
With[{epcc = ϵcc, epco = ϵco},
 surfaceGrad = Compile[{{point, _Real, 1}, {opentr, _Real, 3},
    {normalO, _Real, 2}, {closedtr, _Real, 3}, {normalC, _Real, 2}},
   Block[{ptTri, source = point, normal, u1, u2, cross,
     openS = {0., 0., 0.}, closedS = {0., 0., 0.}},
    Do[
     ptTri = opentr〚i〛;
     normal = normalO〚i〛;
     {u1, u2} = {ptTri〚2〛, ptTri〚-1〛};
     cross = Cross[normal, u2 - u1];
     openS += (0.5 * cross), {i, Length@normalO}
    ];
    Do[
     ptTri = closedtr〚j〛;
     normal = normalC〚j〛;
     {u1, u2} = {ptTri〚2〛, ptTri〚-1〛};
     cross = Cross[normal, u2 - u1];
     closedS += (0.5 * cross), {j, Length@normalC}
    ];
    epcc * closedS + epco * openS
   ], CompilationTarget → "C", RuntimeOptions → "Speed",
   CompilationOptions →
    {"ExpressionOptimization" → True, "InlineExternalDefinitions" → True}]
]
```

Out[*]= CompiledFunction[Argument count: 5
Argument types: {{_Real, 1}, {_Real, 3}, {_Real, 2}, {_Real, 3}, {_Real, 2}}]

In[*]:=
```
CompilePrint[surfaceGrad]
```

Out[*]=
```
5 arguments
1 Boolean register
9 Integer registers
3 Real registers
18 Tensor registers
Underflow checking off
Overflow checking off
Integer overflow checking off
RuntimeAttributes -> {}

T(R1)0 = A1
T(R3)1 = A2
T(R2)2 = A3
```

```
    T(R3)3 = A4
    T(R2)4 = A5
    I3 = 0
    R1 = 1.
    T(R1)6 = {0., 0., 0.}
    R2 = 0.7
    I5 = 2
    I6 = -1
    I8 = 1
    R0 = 0.5
    Result = T(R1)16

1   T(R1)11 = CopyTensor[ T(R1)0]]
2   T(R1)10 = CopyTensor[ T(R1)6]]
3   T(R1)9 = CopyTensor[ T(R1)6]]
4   I2 = Length[ T(R2)2]
5   I4 = I3
6   goto 26
7   T(R2)8 = Part[ T(R3)1, I4]
8   T(R1)5 = Part[ T(R2)2, I4]
9   T(R1)7 = Part[ T(R2)8, I5]
10  T(R1)14 = Part[ T(R2)8, I6]
11  T(R2)12 = {T(R1)7, T(R1)14}
12  I7 = Length[ T(R2)12]
13  B0 = I7 == I5
14  B0 = ! B0
15  if[ !B0] goto 18
16  Return Error
17  goto 18
18  T(R1)7 = GetElement[ T(R2)12, I8]
19  T(R1)14 = GetElement[ T(R2)12, I5]
20  T(R1)12 = - T(R1)7
21  T(R1)15 = T(R1)14 + T(R1)12
22  T(R1)12 = Cross[ T(R1)5, T(R1)15]]
23  T(R1)15 = R0 * T(R1)12
24  T(R1)16 = T(R1)10 + T(R1)15
25  T(R1)10 = CopyTensor[ T(R1)16]]
26  if[ ++ I4 <= I2] goto 7
27  I2 = Length[ T(R2)4]
28  I4 = I3
29  goto 54
30  T(R2)16 = Part[ T(R3)3, I4]
31  T(R2)8 = CopyTensor[ T(R2)16]]
32  T(R1)16 = Part[ T(R2)4, I4]
33  T(R1)5 = CopyTensor[ T(R1)16]]
34  T(R1)16 = Part[ T(R2)8, I5]
35  T(R1)15 = Part[ T(R2)8, I6]
```

```
36    T(R2)17 = {T(R1)16, T(R1)15}
37    I7 = Length[ T(R2)17]
38    B0 = I7 == I5
39    B0 = ! B0
40    if[ !B0] goto 43
41    Return Error
42    goto 43
43    T(R1)16 = GetElement[ T(R2)17, I8]
44    T(R1)7 = CopyTensor[ T(R1)16]]
45    T(R1)16 = GetElement[ T(R2)17, I5]
46    T(R1)14 = CopyTensor[ T(R1)16]]
47    T(R1)17 = - T(R1)7
48    T(R1)16 = T(R1)14 + T(R1)17
49    T(R1)17 = Cross[ T(R1)5, T(R1)16]]
50    T(R1)12 = CopyTensor[ T(R1)17]]
51    T(R1)17 = R0 * T(R1)12
52    T(R1)16 = T(R1)9 + T(R1)17
53    T(R1)9 = CopyTensor[ T(R1)16]]
54    if[ ++ I4 <= I2] goto 30
55    T(R1)16 = R1 * T(R1)9
56    T(R1)17 = R2 * T(R1)10
57    T(R1)16 = T(R1)16 + T(R1)17
58    Return
```

volumetric ∇

In[∘]:=

```
Clear@volumeGrad;
volumeGrad::Information = "volumeGrad computes the volume gradient about a point";
volumeGrad[normalsAssoc_, cellids_, assocTri_, polyhedVols_, growingCellIds_] :=
  Block[{celltopology, gradV, vol, growindkeys, inters},
   gradV = With[{nA = normalsAssoc, aT = assocTri},
     Table[
      celltopology = aT[cell];
      (1. / 3.) Total[(areaTriFn[#] × nA[#]) & /@ celltopology ], {cell, cellids}]
    ];
   vol = AssociationThread[cellids → ConstantArray[Vo, Length@cellids]];
   inters = Intersection[cellids, growingCellIds];
   growindkeys = If[inters ≠ {}, Replace[inters, k_Integer :→ {Key[k]}, {1}], {}];
   vol = Values@If[growindkeys ≠ {}, MapAt[(1 + Vgrowth time) # &, vol, growindkeys], vol];
   Total[(kcv / vol) (polyhedVols / vol - 1) gradV]
  ];
```

vertex ∇

In[ ]:=
```
Clear@gradientVertex;
gradientVertex::Information =
  "determines the sum of the gradients of all the potentials about a vertex";
gradientVertex[ind_, indToPtsAssoc_, triDistAssoc_, vertTriNormalpairings_,
   associatedtri2_, topoF_, polyhedVol_] := Block[{sgterm, vgterm,
    opentri, closetri, normO, normC, pt, triAssoc, normalAssoc, keys, assocTri, polyvol},
   pt = indToPtsAssoc[ind];
   triAssoc = triDistAssoc[ind];
   normalAssoc = vertTriNormalpairings[ind];
   keys = Keys@First@topoF[ind];
   assocTri = associatedtri2[ind];
   polyvol = Lookup[polyhedVol, keys];
   {opentri, closetri} = {triAssoc[1], triAssoc[2]};
   closetri = DeleteDuplicatesBy[closetri, Apply[orderlessHead]];
   {normO, normC} = {Lookup[normalAssoc, opentri], Lookup[normalAssoc, closetri]};
   opentri = rotateSourceVertOrderFn[pt, opentri];
   closetri = rotateSourceVertOrderFn[pt, closetri];
   sgterm = surfaceGrad[pt, opentri, normO, closetri, normC];
   vgterm = volumeGrad[normalAssoc, keys, assocTri, polyvol, growingcellIndices];
   - (vgterm + sgterm)
  ];
```

pair boundary points for computing ∇

In[ ]:=
```
With[{xlim1 = xLim⟦1⟧, xlim2 = xLim⟦2⟧, ylim1 = yLim⟦1⟧, ylim2 = yLim⟦2⟧},
  Clear@boundaryPtsPairing;
  boundaryPtsPairing::Information =
   "the function pairs the points at the boundaries with
     corresponding mirror points";
  boundaryPtsPairing[vertexToCell_, indToPtsAssoc_, ptsToIndAssoc_] := Block[{outerpts,
     mirrorpairs, pt, posits, boundarypts, mirror, keys = Keys[ptsToIndAssoc], fpos},
    outerpts = Keys@Select[vertexToCell, Length[#] ≠ 3 &];
    mirrorpairs = <|
       (pt = Lookup[indToPtsAssoc, #];
          If[
           pt⟦1⟧ ≤ xlim1 || pt⟦1⟧ ≥ xlim2 || pt⟦2⟧ ≤ ylim1 || pt⟦2⟧ ≥ ylim2,
           mirror = Lookup[ptsToIndAssoc, {pt /. periodicRules},
             (fpos = With[{insert = pt /. periodicRules},
                 FirstPosition[Chop[# - insert & /@ keys, 10^-5], {0, 0, 0}]
                ];
              ptsToIndAssoc[Extract[keys, fpos]])
            ];
           # → mirror,
           Nothing]) & /@ outerpts
       |> // KeySort;
    boundarypts =
     Map[Sort@*Flatten][List @@@ Normal@GroupBy[Normal@mirrorpairs, Last → First]];
    (*(*option 1:*)
    DeleteDuplicates[ReverseSortBy[boundarypts,Length],Length[#1⋂#2]==2&];*)
    (*option 2:*)
    posits = Position[boundarypts, x_ /; Length[x] == 3];
    Complement[boundarypts,
     Flatten[Map[Permutations[#, {2}] &, Extract[boundarypts, posits]], 1]
    ]
   ]
 ];
```

integrating mesh

In[◦]:=
```
Clear@adjustGrad;
adjustGrad::Information =
  "the function ensures that the boundary points and their mirror
    points have the same gradient";
adjustGrad[grad_, bptpairs_] := Block[{vals, g = grad},
   Scan[
    keys ↦ (
      vals = SetPrecision[Mean@Lookup[grad, keys], 8];
      Scan[(g[#] = vals) &, keys]
     ), bptpairs];
   g
  ];
```

paramFinder

In[◦]:=
```
With[{faceorientedQ = OptionValue[paramFinder, "OrientedFaces"]},
  paramFinder[indToPtsAssoc_, $CVG_, keyslocaltopo_, shiftVecAssoc_,
    vertKeys_, OptionsPattern[]] := Block[{$faceListAssoc, $topo,
     localtrimesh, tempassoc = <||>, meshed, $assoctri, trimesh, polyhed,
     polyhedcent, $polyhedVol, cellcent, normals, normNormals,
     centTri, signednormals, $vertTriNormpair, opencloseTri,
     $triDistAssoc, trianglemembers, ckeys, signs, dim},
    (*Adjust params for the the new geometry M-X*)
    $faceListAssoc = Map[Lookup[indToPtsAssoc, #] &, $CVG, {2}];
    $topo = cellTranslator[$faceListAssoc, keyslocaltopo, shiftVecAssoc, vertKeys];
    $assoctri = With[{keys = Keys[indToPtsAssoc]},
      SetPrecision[
       AssociationThread[keys,
        Table[Map[Splice@Partition[#, 3] &@localTriFunc[#, indToPtsAssoc[i]] &,
          $topo[i][[1]], {2}], {i, keys}]], 8]
     ];
    opencloseTri = Flatten[Values@#, 1] & /@ $assoctri;
    (*trimesh=triangulateToMesh/@$faceListAssoc;*)
    trimesh = Map[tToMesh, $faceListAssoc, {2}];
    If[faceorientedQ,
     $polyhedVol = volumePolyhedra /@ trimesh;
     polyhedcent = <|
       KeyValueMap[#1 → centroidPolyhedra[#2, $polyhedVol[#1]] &, trimesh]|>,
     (*else*)
     polyhed = Polyhedron@* (Flatten[#, 1] &) /@ trimesh;
     ckeys = Keys@trimesh;
     {polyhedcent, $polyhedVol} =
```

```
      AssociationThread[ckeys, #] & /@ parPolyhedProp[polyhed]
     (*
     polyhedcent=RegionCentroid/@polyhed;
     $polyhedVol=AssociationThread[Keys[polyhed]→Volume[Values@polyhed]]
     *)
    ];
    (*cellcent=cellCentroids[polyhedcent,keyslocaltopo,shiftVecAssoc];*)
    normals = Values /@ Map[triNormal, $assoctri, {3}];
    normNormals = Map[normNormal, normals, {3}];
    signednormals = normNormals;
    (*centTri=Map[SetPrecision[#,8]&,<|#→meanTri[Values[$assoctri@#]]&/@vertKeys|>];
    (*normNormals=Map[Normalize,normals,{3}];*)
    signednormals=AssociationThread[vertKeys,
      Map[
       MapThread[
         #2 Sign@MapThread[Function[{x,y},(y-#1).x],{#2,#3}]&,
         {cellcent[#],normNormals[#],centTri[#]}]&,vertKeys]];
    *)
    If[Not@faceorientedQ,
     centTri =
      Map[SetPrecision[#, 8] &, <|# → meanTri[Values[$assoctri@#]] & /@ vertKeys|>];
     signs = AssociationThread[Keys@indToPtsAssoc,
       Map[
        MapThread[
          Sign@MapThread[Function[{x, y}, (y - #1).x], {#2, #3}] &,
          {cellcent[#], normNormals[#], centTri[#]}] &, vertKeys]
      ];
     opencloseTri = MapThread[MapAt[Function[coords, {coords[[1]], coords[[3]], coords[[2]]}],
         #1, Position[Flatten[#2, 1], -1]] &, {opencloseTri, signs}];
     $assoctri = AssociationThread[
       vertKeys → MapThread[
          (dim = Values[Map[Length][#1]];
            AssociationThread[Keys[#1] → TakeList[#2, dim]]) &,
          {$assoctri, opencloseTri}]
      ];
    ];
    $vertTriNormpair = <|
      # → <|Thread[opencloseTri[#] → Flatten[signednormals@#, 1]]|> & /@ vertKeys|>;
    $triDistAssoc = (GroupBy[GatherBy[#, Intersection], Length, Flatten[#, 1] &]) & /@
      opencloseTri;
    {$triDistAssoc, $vertTriNormpair, $assoctri, $topo, $polyhedVol}
   ]
  ];
```

Integrator

In[∘]:=
```
Clear@RK4Integrator;
RK4Integrator::Information = "the module comprises
```

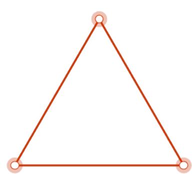
```
    the Runge-Kutta Order 5 (RK5) scheme for integrating the mesh";
RK4Integrator[indToPtsAssoc_, topo_, cellVertG_, $vertexToCell_, ptsToIndAssoc_] :=
  Block[{grad1, grad2, grad3, grad4, grad5, grad6, $indToPtsAssoc = indToPtsAssoc,
    $triDistAssoc, $vertTriNormpair, $assoctri, $topo = topo, $polyhedVol,
    $CVG = cellVertG, shiftVecAssoc, keyslocaltopo, vertKeys = Keys@indToPtsAssoc,
    $indToPtsAssocOrig = indToPtsAssoc, bptpairs, vals},
   (*computed once at the start of the computation*)
   keyslocaltopo = Keys@*First /@ topo;
   shiftVecAssoc = Association /@
     Map[Apply[Rule], Thread /@ Select[(#[[2 ;; 3]]) & /@ topo, # ≠ {{}, {}} &], {2}];
   bptpairs = boundaryPtsPairing[$vertexToCell, indToPtsAssoc, ptsToIndAssoc];
   (*If[time==1*δt ||time==2δt||time==3*δt ,Print@bptpairs];*)
   {$triDistAssoc, $vertTriNormpair, $assoctri, $topo, $polyhedVol} =
    paramFinder[$indToPtsAssoc, $CVG, keyslocaltopo, shiftVecAssoc, vertKeys];
   (*compute the gradient of the original mesh M1 *)
   grad1 = AssociationThread[vertKeys,
     SetPrecision[Table[gradientVertex[i, $indToPtsAssoc,
        $triDistAssoc, $vertTriNormpair, $assoctri, $topo, $polyhedVol],
       {i, vertKeys}], 8]];
   grad1 = adjustGrad[grad1, bptpairs];
   (*displace vertices by the numerical gradient*)
   $indToPtsAssoc = <|
     KeyValueMap[#1 → SetPrecision[#2 + 0.5 grad1[#1] δt, 8] &, $indToPtsAssocOrig] |>;
   (*adjust and compute params for the intermediate geometry M2*)
   {$triDistAssoc, $vertTriNormpair, $assoctri, $topo, $polyhedVol} =
    paramFinder[$indToPtsAssoc, $CVG, keyslocaltopo, shiftVecAssoc, vertKeys];
   (*compute the gradient for M2*)
   grad2 = AssociationThread[vertKeys,
     SetPrecision[Table[gradientVertex[i, $indToPtsAssoc,
        $triDistAssoc, $vertTriNormpair, $assoctri, $topo, $polyhedVol],
       {i, vertKeys}], 8]];
   grad2 = adjustGrad[grad2, bptpairs];
   (*displace vertices by the numerical gradient*)
   $indToPtsAssoc = <|
     KeyValueMap[#1 → SetPrecision[#2 + 0.5 (grad2[#]) δt, 8] &, $indToPtsAssocOrig] |>;
   (*adjust and compute params for the intermediate geometry M3*)
   {$triDistAssoc, $vertTriNormpair, $assoctri, $topo, $polyhedVol} =
    paramFinder[$indToPtsAssoc, $CVG, keyslocaltopo, shiftVecAssoc, vertKeys];
   (*compute the gradient for M3*)
   grad3 = AssociationThread[vertKeys,
     SetPrecision[Table[gradientVertex[i, $indToPtsAssoc,
        $triDistAssoc, $vertTriNormpair, $assoctri, $topo, $polyhedVol],
       {i, vertKeys}], 8]];
   grad3 = adjustGrad[grad3, bptpairs];
   (*displace vertices by the numerical gradient*)
   $indToPtsAssoc = <|
     KeyValueMap[#1 → SetPrecision[#2 + (grad3[#]) δt, 8] &, $indToPtsAssocOrig] |>;
```

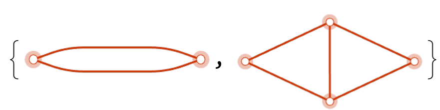
```
 (*adjust and compute params for the intermediate geometry M4*)
 {$triDistAssoc, $vertTriNormpair, $assoctri, $topo, $polyhedVol} =
  paramFinder[$indToPtsAssoc, $CVG, keyslocaltopo, shiftVecAssoc, vertKeys];
 (*compute the gradient for M4*)
 grad4 = AssociationThread[vertKeys,
   SetPrecision[Table[gradientVertex[i, $indToPtsAssoc,
      $triDistAssoc, $vertTriNormpair, $assoctri, $topo, $polyhedVol],
     {i, vertKeys}], 8]];
 grad4 = adjustGrad[grad4, bptpairs];
 (*displace vertices by the numerical gradient*)
 $indToPtsAssoc = Map[SetPrecision[#, 8] &][<|
    KeyValueMap[#1 → #2 + (1. / 6) (grad1[#1] + 2. grad2[#] + 2. grad3[#] + grad4[#]) δt &,
     $indToPtsAssocOrig] |>]
];
```

topological network operations [Δ<>I] ∧ [I<>Δ]

checks to determine whether α, β, γ or an invalid pattern is present in the graph

In[∘]:=
```
$invalidPatternsEdge = Graph[{1 ⟷ 2, 2 ⟷ 3, 3 ⟷ 1}];
Echo[Graph[$invalidPatternsEdge, PlotTheme → "Web", ImageSize → Tiny],
  Style["invalid pattern (edge in Δ): ", Black]];
$invalidPatterns = {
   Graph[{1 ⟷ 2, 2 ⟷ 1}],
   Graph[{1 ⟷ 2, 2 ⟷ 3, 3 ⟷ 1, 1 ⟷ 4, 3 ⟷ 4}]
  };
Echo[Graph[#, PlotTheme → "Web", ImageSize → Tiny] & /@ $invalidPatterns,
  Style["invalid pattern (double edge || double Δ): ", Black]];
```

» invalid pattern (edge in Δ): 

» invalid pattern (double edge || double Δ): 

In[∘]:=
```
edgeinTrianglePatternQ[graph_] := IGSubisomorphicQ[$invalidPatternsEdge, graph];
InvalidEdgePatternQ[graph_] := AnyTrue[$invalidPatterns, IGSubisomorphicQ[#, graph] &];
InvalidTrigonalPatternQ[graph_] :=
  AnyTrue[$invalidPatterns, IGSubisomorphicQ[#, graph] &];
```

In[ ]:=
```
faceIntersections[polyhed_] := AnyTrue[
   Length /@ (Intersection @@@ Replace[Subsets[Partition[#, 2, 1, 1] & /@ polyhed, {2}],
       List → orderlessHead, {4}, Heads → True]), # ≥ 2 &];

gammaPatternFreeQ[polyhedList_] := Not[Or @@ (faceIntersections /@ polyhedList)];
```

I → Δ operator

In[ ]:=
```
ItoΔpreprocess1::description =
  "the F[x] extracts the vertex pairings from the local topology i.e. {r10,r11}
    and {r1,r4} & {r2,r5} & {r3,r6} → (points attached to r10,r11)";
ItoΔpreprocess1[candidate_, currentTopology_, localTopology_] :=
  Block[{r10, r11, ptsPartitioned, vertAttached ,
    cellsPartOf, cellsElim, ptsAttached},
   {r10, r11} = candidate; (* edge unpacked into vertices: r10,r11 *)
   (* r10 → {vertices attached with r10}, r11 → {vertices attached with r11} *)
   ptsPartitioned = If[Keys[#],
       r10 → Flatten[Last@#, 1], r11 → Flatten[Last@#, 1]] & /@ (
      Normal@KeySortBy[
         GroupBy[
          (currentTopology /. {OrderlessPatternSequence[r11, r10]} → Sequence[]),
          MemberQ[#, r10] &], MatchQ[False]] /. {r10 | r11 → Sequence[]});
   (* the code below creates pairings between vertices
    such that r1 is packed with r4, r2 with r5 & r3 with r6 *)
   vertAttached = Flatten[Values@ptsPartitioned, 1];
   cellsPartOf =
    Union[Position[localTopology, #, {3}] /. {Key[x_], __} :→ x] & /@ vertAttached;
   cellsElim = Complement[Union@Flatten[cellsPartOf],
       Union@Flatten@#[[1]] ⋂ Union@Flatten@#[[2]]] &@TakeDrop[cellsPartOf, 3];
   If[cellsElim ≠ {},
    cellsPartOf = cellsPartOf /. Alternatives @@ cellsElim → Sequence[]
   ];
   ptsAttached = Values@GroupBy[Thread[vertAttached → cellsPartOf], Last → First];
   {r10, r11, ptsAttached}
];
```

In[ ]:=
```
Ito△preprocess2::description =
  "the F[x] computes {r7,r8,r9} vertices from the vertices
    attached with r10 & r11 i.e. (r1-r6)";
Ito△preprocess2[ptsAttached_, {r10_, r11_}] :=
  Block[{r01, u1T, r1, r4, r2, r5, r3, r6, w07, w08, w09,
    v07, v08, v09, lmax, r7, r8, r9},
   r01 = Mean[{r10, r11}];
   u1T = (r10 - r11) / Norm[r10 - r11];
   {{r1, r4}, {r2, r5}, {r3, r6}} = ptsAttached;
   w07 = 0.5 ((r1 - r01) / Norm[r1 - r01] + (r4 - r01) / Norm[r4 - r01]);
   w08 = 0.5 ((r2 - r01) / Norm[r2 - r01] + (r5 - r01) / Norm[r5 - r01]);
   w09 = 0.5 ((r3 - r01) / Norm[r3 - r01] + (r6 - r01) / Norm[r6 - r01]);
   v07 = w07 - (w07.u1T) u1T;
   v08 = w08 - (w08.u1T) u1T;
   v09 = w09 - (w09.u1T) u1T;
   lmax = Max[Norm[v08 - v07], Norm[v09 - v08], Norm[v07 - v09]];
   r7 = SetPrecision[r01 + (δ / lmax) v07, 8];
   r8 = SetPrecision[r01 + (δ / lmax) v08, 8];
   r9 = SetPrecision[r01 + (δ / lmax) v09, 8];
   {r1, r2, r3, r4, r5, r6, r7, r8, r9}
];
```

In[ ]:=
```
insertTrigonalFace::description = "the module inserts the trigonal face into the cell";
insertTrigonalFace[topology_, r7_, r8_, r9_, r10_, r11_] := Block[{posInserts},
   posInserts = Position[
     FreeQ[#, {___, OrderlessPatternSequence[r10, r11], ___}] & /@ topology, True];
   If[posInserts ≠ {},
    Insert[topology, {r7, r8, r9}, Flatten[{#, -1}] & /@ posInserts],
    topology]
  ];
```

In[ ]:=
```
Clear@corrTriOrientationHelper;
corrTriOrientationHelper[topology_, trigonalface_] :=
  Block[{allTri, selectTriAttached, selectTriSharedEdge, selectTri,
    partTri, partAttachedTri},
   partTri = Partition[trigonalface, 2, 1, 1];
   allTri = Flatten[triangulateToMesh@topology, 1];
   selectTriAttached =
    Cases[allTri, {OrderlessPatternSequence[__, Alternatives @@ trigonalface]}];
   selectTriSharedEdge = Select[selectTriAttached,
     Length[Intersection[#, trigonalface]] == 2 &];
   selectTri = RandomChoice@selectTriSharedEdge;
   partAttachedTri = Partition[selectTri, 2, 1, 1];
   If[Intersection[partAttachedTri, partTri] ≠ {},
    topology /. trigonalface :→ Reverse@trigonalface,
    topology
   ]
  ];
```

In[ ]:=
```
Clear@corrTriOrientation;
corrTriOrientation::description =
  "the function corrects the orientation of the added trigonal
    face, such that it is oriented c.c.w";
corrTriOrientation[localtopology_, trigonalface_] := Block[{cells, affectedIDs, topo},
   cells = Map[DeleteDuplicates@*(Flatten[#, 1] &), localtopology, {2}];
   affectedIDs = Partition[First /@ Position[cells, trigonalface], 1];
   topo = MapAt[corrTriOrientationHelper[#1, trigonalface] &, cells, affectedIDs];
   Map[Partition[#, 2, 1, 1] &, topo, {2}]
  ];
```

In[ ]:=
```
ItoΔoperation::description =
  "the module removes vertices r10,r11 and connects the points
    r1-r6 with the new points r7-r9";
ItoΔoperation[graphnewLocalTopology_, cellCoords_, r1_, r2_, r3_, r4_,
   r5_, r6_, r7_, r8_, r9_, r10_, r11_] := Block[{mat},
    mat = insertTrigonalFace[cellCoords, r7, r8, r9, r10, r11];
    Map[Partition[#, 2, 1, 1] &, mat, {2}] /. {
      {OrderlessPatternSequence[r11, r10]} :> Sequence[],
      {PatternSequence[r11, q : r4 | r5 | r6]} :>
       Switch[q, r4, {r7, r4}, r5, {r8, r5}, r6, {r9, r6}],
      {PatternSequence[q : r4 | r5 | r6], r11} :>
       Switch[q, r4, {r4, r7}, r5, {r5, r8}, r6, {r6, r9}],
      {PatternSequence[r10, q : r1 | r2 | r3]} :>
       Switch[q, r1, {r7, r1}, r2, {r8, r2}, r3, {r9, r3}],
      {PatternSequence[q : r1 | r2 | r3, r10]} :>
       Switch[q, r1, {r1, r7}, r2, {r2, r8}, r3, {r3, r9}]}
   ] /; (! InvalidEdgePatternQ[graphnewLocalTopology]);
```

In[ ]:=
```
bindCellsToNewTopology::description =
  "the module pairs modified cell topologies with cell IDs if 'γ' pattern is absent";
bindCellsToNewTopology[adjoiningCells_, network_, func_ : Identity] /;
   gammaPatternFreeQ[network] := Thread[adjoiningCells → func[network]];
```

In[ ]:=
```
modifier::description = "the module makes
    modifications to the datastructures after topological transitions";
modifier[candidate_, adjoiningCells_, indToPtsAssoc_,
   ptsToIndAssoc_, cellVertexGrouping_,
vertexToCell_, celltopologicalChanges_, updatedLocalNetwork_, newAdditions_] :=
  Block[{dropVertInds, $ptsToIndAssoc = ptsToIndAssoc,
    $indToPtsAssoc = indToPtsAssoc, $cellVertexGrouping = cellVertexGrouping,
    $vertexToCell = vertexToCell},
   dropVertInds = Lookup[$ptsToIndAssoc, candidate];
   KeyDropFrom[$ptsToIndAssoc, candidate];
   KeyDropFrom[$indToPtsAssoc, dropVertInds];
   {AssociateTo[$ptsToIndAssoc, #~Reverse~2], AssociateTo[$indToPtsAssoc, #]} &@
    newAdditions;
   AssociateTo[$cellVertexGrouping, MapAt[$ptsToIndAssoc,
     celltopologicalChanges, {All, 2, All, All}]];
   KeyDropFrom[$vertexToCell, Sort@dropVertInds];
   AssociateTo[$vertexToCell,
    (First[#] → Part[adjoiningCells, Union[
          First /@ Position[updatedLocalNetwork, Last@#, {3}]]]) & /@ newAdditions];
   {$indToPtsAssoc, $ptsToIndAssoc, $cellVertexGrouping, $vertexToCell}
  ];
```

In[ ]:=
```
ItoΔ[edges_, faceListCoords_, indToPtsAssoc_,
   ptsToIndAssoc_, cellVertexGrouping_, vertexToCell_, wrappedMat_] :=
```

```
Block[{edgelen, edgesel, candidate, graphCurrentTopology, currentTopology, z, ž,
  localtopology = {}, adjoiningcells, cellCoords, r10, r11, ptsAttached, r1, r2, r3,
  r4, r5, r6, r7, r8, r9, newLocalTopology, graphnewLocalTopology, modifiednetwork,
  cellTopologicalChanges, maxVnum, wrappedcells, celltransvecAssoc, newAdditions,
  transvec, ls, vpt, cellTopologicalChangesBeforeShift, positions, cellspartof,
  vertices, $indToPtsAssoc = indToPtsAssoc, $ptsToIndAssoc = ptsToIndAssoc,
  $cellVertexGrouping = cellVertexGrouping, $vertexToCell = vertexToCell,
  $edges = edges, $wrappedMat = wrappedMat, $faceListCoords = faceListCoords},

 edgelen = lenEdge @@@ $edges; (*here we check the length of all the edges,
 we can also use built-in EuclideanDistance[]*)
 edgesel = Pick[$edges, 1 - UnitStep[edgelen - δ], 1];
 (*select edges that have length less than critical value δ*)
 Scan[
  (candidate = #; (*candidate edge*)
    vertices = DeleteDuplicates@Flatten[$edges, 1];
    If[AllTrue[candidate, MemberQ[vertices, #] &],
     (*this means that the edge exists in the network.
        If there are two adjacent edges
      that need to be transformed and one gets transformed first
      then the second one will not exist*)
     (* get all edges that are connected to our edge of interest *)
     currentTopology = Cases[$edges,
       {OrderlessPatternSequence[x_, p : Alternatives @@ candidate]} :> {p, x}];
     (* this part of code takes care of border cells *)
     If[Length[currentTopology] < 7,
      (*Print[" # of edges is < than 7 "];*)
      (* here we get the local topology of our network *)
      {localtopology, wrappedcells, transvec} =
       getLocalTopology[$ptsToIndAssoc, $indToPtsAssoc, $vertexToCell,
         $cellVertexGrouping, $wrappedMat, $faceListCoords][candidate];
      (*Print[Keys@localtopology];*)
      (* this yields all the unique edges
       in the localtopology and extract vertex pairs, such that
       {candidate_vertex, vertex attached to candidate} *)
      With[{edg = DeleteDuplicatesBy[
          Flatten[Map[Partition[#, 2, 1, 1] &, Values@localtopology, {2}], 2], Sort]},
       currentTopology = Cases[edg,
          {OrderlessPatternSequence[x_, p : Alternatives @@ candidate]} :> {p, x}];
      ];
     ];
     (*creating a graph from the current topology*)
     graphCurrentTopology =
      Graph@Replace[currentTopology, List → UndirectedEdge, {2}, Heads → True];
     If[edgeinTrianglePatternQ@graphCurrentTopology,
      (*edge is part of a trigonal face and
       hence nothing is to be done. this prevents `α` pattern *)
```

```
None,
{z, ž} = candidate; (* edge vertices unpacked *)
If[localtopology == {},
  (* here we get the local topology of our network *)
 {localtopology, wrappedcells, transvec} =
   getLocalTopology[$ptsToIndAssoc, $indToPtsAssoc, $vertexToCell,
     $cellVertexGrouping, $wrappedMat, $faceListCoords][candidate];
];
{adjoiningcells, cellCoords} = {Keys@#, Values@#} &@localtopology;
(* adjoining cells and their vertices *)
(*Print[adjoiningcells];*)
(* label vertices joining the candidate edge *)
{r10, r11, ptsAttached} =
 ItoΔpreprocess1[candidate, currentTopology, localtopology];
(* getting all vertices for transformation including (r7,r8,r9) *)
{r1, r2, r3, r4, r5, r6, r7, r8, r9} = ItoΔpreprocess2[ptsAttached, {r10, r11}];
(*
(*print old and predicted topology *)
Print[
  Graphics3D[{PointSize[0.025],Red,Point@{r1,r4,r7},
    Green,Point@{r2,r5,r8},Blue,Point@{r3,r6,r9},Purple,
    Point@r10,Pink,Point@r11,Black,Line@currentTopology,Dashed,
    Line[{r1,r7}],Line[{r4,r7}],Line[{r2,r8}],Line[{r5,r8}],
    Line[{r3,r9}],Line[{r6,r9}],Purple,Line@ptsAttached},ImageSize→Small]
 ];
*)
If[! IGSubisomorphicQ[$invalidPatternsEdge, graphCurrentTopology],
 (* atleast no α pattern will be generated. I think
  this has been checked in the If statement prior to this *)
 (* Scheme: apply [I]→[H]; check if the new topology is valid (i.e. no α,β);
 check if the new topology is free of γ pattern;
 replace network architecture *)
 (*forming new topology and graph*)
 newLocalTopology = {r1 ⟷ r7, r4 ⟷ r7,
   r2 ⟷ r8, r5 ⟷ r8, r3 ⟷ r9, r6 ⟷ r9, r7 ⟷ r8, r8 ⟷ r9, r9 ⟷ r7};
 graphnewLocalTopology = Graph@newLocalTopology;
 (* apply ItoΔ operation *)
 modifiednetwork = ItoΔoperation[graphnewLocalTopology,
   cellCoords, r1, r2, r3, r4, r5, r6, r7, r8, r9, r10, r11];
 modifiednetwork = corrTriOrientation[modifiednetwork, {r7, r8, r9}];
 (*bind cells with their new topology if γ pattern is absent*)
 cellTopologicalChanges = bindCellsToNewTopology[adjoiningcells,
   modifiednetwork, Map[Map[DeleteDuplicates@Flatten[#, 1] &]]];
 (*
 (*print topology post operation *)
 If[(cellTopologicalChanges≠{})||
    (Head[cellTopologicalChanges]=!=bindCellsToNewTopology),
```

```
Print[ind→Graphics3D[{{Opacity[0.1],Blue,Polyhedron/@
        Values[cellTopologicalChanges]},
      {Red,Line@candidate}},Axes→True]]
 ];
*)
If[(cellTopologicalChanges ≠ {}) ||
  (Head[cellTopologicalChanges] =!= bindCellsToNewTopology),
 (*if you are here then it means that cell topology was altered *)
 modifiednetwork = Values@cellTopologicalChanges;
 (*vertex coordinates of the modified topology*)
 maxVnum = Max[Keys@$indToPtsAssoc]; (*maximum
  number of vertices so far*)
 If[wrappedcells ≠ {},
  (* if there are wrapped
   cells send them back to their respective positions *)
  (* wrapped cells with their respective vectors for translation *)
  celltransvecAssoc = AssociationThread[wrappedcells, transvec];
  cellTopologicalChangesBeforeShift = cellTopologicalChanges;
  (* here we send the cells
    back to their original positions → unwrapped state *)
  cellTopologicalChanges = (x ↦ With[{p = First[x]},
       If[MemberQ[wrappedcells, p],
        p → Map[SetPrecision[# - celltransvecAssoc[p], 8] &, Last[x], {2}], x]
      ]) /@ cellTopologicalChanges;

  ls = {};
  Scan[
   vpt ↦
    (positions = Position[cellTopologicalChangesBeforeShift, vpt];
     positions = DeleteDuplicates[{First[#]} & /@ positions];
     cellspartof = Extract[adjoiningcells, positions];
     Fold[
      Which[MemberQ[wrappedcells, #2],
        AppendTo[ls, SetPrecision[vpt - celltransvecAssoc[#2], 8] ],
        True, If[! MemberQ[ls, vpt], AppendTo[ls, vpt]]] &, ls, cellspartof]),
   {r7, r8, r9}];

  newAdditions = Thread[(Range[Length@ls] + maxVnum) → ls],
  newAdditions = Thread[(Range[3] + maxVnum) → {r7, r8, r9}]
  (* labels for new vertices *)
 ];

 (* appropriate changes are made to the datastruct *)
 {$indToPtsAssoc, $ptsToIndAssoc, $cellVertexGrouping, $vertexToCell} =
  modifier[candidate, adjoiningcells, $indToPtsAssoc,
   $ptsToIndAssoc, $cellVertexGrouping,
   $vertexToCell, cellTopologicalChanges, modifiednetwork, newAdditions];
```

```
          $faceListCoords = Map[Lookup[$indToPtsAssoc, #] &, $cellVertexGrouping, {2}];

          $edges =
           Flatten[Map[Partition[#, 2, 1, 1] &, Map[Lookup[$indToPtsAssoc, #] &, Values[
                $cellVertexGrouping], {2}], {2}], 2] // DeleteDuplicatesBy[Sort];

          $wrappedMat = With[{temp = Keys[$cellVertexGrouping]},
            AssociationThread[temp → Map[Lookup[$indToPtsAssoc, #] /. periodicRules &,
               Lookup[$cellVertexGrouping, temp], {2}]]
           ];
         ];
        ];
       ];
      ]) &, edgesel];
   {$edges, $indToPtsAssoc,
    $ptsToIndAssoc, $cellVertexGrouping, $vertexToCell, $wrappedMat}
  ];
```

Δ → I operator

In[∘]:=

```
pickTriangulatedFaces::description = "pick candidate Δ faces to transform";
pickTriangulatedFaces[faceListCoords_] :=
  Block[{triangleCandidates, triangleCandidatesSel},
   triangleCandidates = Cases[faceListCoords, x_ /; Length[x] == 3, {2}];
   (* yield all Δ faces from the mesh & retain
    those that pass Satoru's 2nd condition *)triangleCandidatesSel =
    AllTrue[lenEdge @@@ Partition[#, 2, 1, 1], # ≤ δ &] & /@ triangleCandidates;
   Pick[triangleCandidates, triangleCandidatesSel, True]
  ];
```

In[∘]:=

```
ΔtoIoperation[network_, rules_] := Block[{ruleapply},
   ruleapply =
    ((network /. rules) /. Line[] → Sequence[]) /. {Line → Sequence, {} → Sequence[]};
   Map[DeleteDuplicates@Flatten[#, 1] &, ruleapply, {2}]
  ];
```

In[∘]:=
```
rulesΔtoI[currentTopology_, ptsTri_, ptPartition_] :=
  Block[{attachedEdges, triedges, reconnectRules, rules},
    (*edges connected with face*)
    attachedEdges = DeleteCases[currentTopology,
      Alternatives @@ ({OrderlessPatternSequence @@ #} & /@ Partition[ptsTri, 2, 1, 1])];
    triedges = Complement[currentTopology, attachedEdges];
    (* only edges that form the trigonal face *)
    reconnectRules = Flatten[Cases[attachedEdges,
         q : {y_, p : Alternatives @@ Last[#]} :→ q → {First@#, p}] & /@ ptPartition];
    rules = Dispatch[reconnectRules~Join~Reverse[reconnectRules, {3}]~Join~(
        {OrderlessPatternSequence @@ #} → Sequence[] & /@ triedges)];
    rules
   ] /; (! InvalidTrigonalPatternQ[
      Graph@Replace[currentTopology, List → UndirectedEdge, {2}, Heads → True]]);
```

In[∘]:=
```
ΔtoIpreprocess[ptsTri_, currentTopology_] :=
  Block[{sortptsTri, uTH, r1, r2, PtsAcrossFaces,
    ptsAttached, newPts, ptPartition, newLocalTopology, vec},
   With[{r0H = Mean@ptsTri},
    sortptsTri = SortBy[ptsTri, ArcTan[# - r0H] &];
    (* arrange the points in an clockwise || anti-clockwise manner *)uTH = Function[
       Cross[#2 - #1, #3 - #1] / (Norm[#2 - #1] Norm[#3 - #1])][Sequence @@ sortptsTri];
    r1 = SetPrecision[r0H + 0.5 δ * uTH, 8];
    r2 = SetPrecision[r0H - 0.5 δ * uTH, 8];
    vec = Normalize[r1 - r2];
    ptsAttached = DeleteCases[currentTopology~Flatten~1, Alternatives @@ ptsTri];
    (* are points above or below the Δ *)
    PtsAcrossFaces = GroupBy[ptsAttached, Sign[vec.(r0H - #)] &];
    (* compute the 2 new pts from the trio of old pts *)
    newPts = <|Sign[vec.(r0H - #)] → # & /@ {r1, r2}|>;
    ptPartition = Values@Merge[{newPts, PtsAcrossFaces}, Identity];
    (* which points belong with r1 and which points with r2 *)newLocalTopology =
     Flatten[Map[x ↦ First[x] ⟷ # & /@ Last[x], ptPartition], 1]~Join~{r1 ⟷ r2};
    {ptPartition, newLocalTopology, r1, r2}]
  ];
```

In[∘]:=
```
ΔtoI[edges_, faceListCoords_, indToPtsAssoc_,
   ptsToIndAssoc_, cellVertexGrouping_, vertexToCell_, wrappedMat_] :=
  Block[{selectTriangle, candidate, currentTopology, ptsAttached, graphCurrentTopology,
    ptsTri, PtPartition, newLocalTopology, adjoiningCells, prevNetwork,
    updatedLocalNetwork, rules, celltopologicalChanges, r1, r2, maxVnum, newAdditions,
    localtopology, wrappedcells, transvec, cellCoords, ls, positions, celltransvecAssoc,
    cellTopologicalChangesBeforeShift, cellspartof, $faceListCoords = faceListCoords,
    $ptsToIndAssoc = ptsToIndAssoc, $indToPtsAssoc = indToPtsAssoc,
    $vertexToCell = vertexToCell, $cellVertexGrouping = cellVertexGrouping,
```

```
  $wrappedMat = wrappedMat, vpt, $edges = edges, selectTriangles},
 selectTriangles = pickTriangulatedFaces@*Values@$faceListCoords;
 Scan[
  (candidate = #;
    If[And @@ (KeyMemberQ[$ptsToIndAssoc, #] & /@ candidate),
     (* get local network topology from the Δ
      face: basically which coordinates the face is linked to *)
     {localtopology, wrappedcells, transvec} =
      getLocalTopology[$ptsToIndAssoc, $indToPtsAssoc, $vertexToCell,
        $cellVertexGrouping, $wrappedMat, $faceListCoords][candidate];
     {adjoiningCells, cellCoords} = {Keys@#, Values@#} &@localtopology;
     (* adjoining cells and their vertices *)
     prevNetwork = Map[Partition[#, 2, 1, 1] &, cellCoords, {2}];
     (* this yields all the unique edges
      in the current topology and extract vertex pairs, such that
      {candidate_vertex, vertex_attached with candidate} *)
     currentTopology = Cases[DeleteDuplicatesBy[Flatten[prevNetwork, 2], Sort],
       {OrderlessPatternSequence[x_, p : Alternatives @@ candidate]} :→ {p, x}];
     (*creating a graph from the current topology*)
     graphCurrentTopology =
      Graph@Replace[currentTopology, List → UndirectedEdge, {2}, Heads → True];
     If[! InvalidTrigonalPatternQ[graphCurrentTopology],
      (* transform the network topology by applying [H]→[I] operation *)
      ptsTri = candidate; (* vertices of the faces *)
      {PtPartition, newLocalTopology, r1, r2} =
       ΔtoIpreprocess[ptsTri, currentTopology];
      (*Print@Graphics3D[{{Dashed,Thick,Opacity[0.6],Black,Line@currentTopology},
          {Thick,Opacity[0.6],Darker@Blue,
           Line[newLocalTopology/.UndirectedEdge→ List]},
          {Red,PointSize[0.035],Point@PtPartition[[2,-1]]},
          {Blue,PointSize[0.035],Point@PtPartition[[1,-1]]},
          {Orange,PointSize[0.05],Point@candidate},{Darker@Green,
           PointSize[0.05],Point@{r1,r2}}},ImageSize→Small];*)
      rules = rulesΔtoI[currentTopology, ptsTri, PtPartition];
      Switch[
       rules, _rulesΔtoI, None,
       _,
       (updatedLocalNetwork = ΔtoIoperation[prevNetwork, rules];
        celltopologicalChanges = bindCellsToNewTopology[adjoiningCells,
            updatedLocalNetwork] /. _bindCellsToNewTopology → {};
        If[celltopologicalChanges ≠ {},
         (*Print[Graphics3D[
             {{Opacity[0.1],Blue,Polyhedron/@Values[celltopologicalChanges]},
              {Red,Line[candidate~Append~First[candidate]]}},Axes→True]];*)

         maxVnum = Max[Keys@$indToPtsAssoc];
```

```
If[wrappedcells ≠ {},
  (* if there are wrapped
   cells send them back to their respective positions *)
  (* wrapped cells with their respective vectors for translation *)
  celltransvecAssoc = AssociationThread[wrappedcells, transvec];
  cellTopologicalChangesBeforeShift = celltopologicalChanges;
  (* here we send the cells
    back to their original positions → unwrapped state *)
  celltopologicalChanges = (x ↦ With[{p = First[x]},
        If[MemberQ[wrappedcells, p], p →
          Map[SetPrecision[# - celltransvecAssoc[p], 8] &, Last[x], {2}], x]
       ]) /@ celltopologicalChanges;

  ls = {};
  Scan[
   vpt ↦
    (positions = Position[cellTopologicalChangesBeforeShift, vpt];
     positions = DeleteDuplicates[{First[#]} & /@ positions];
     cellspartof = Extract[adjoiningCells, positions];
     Fold[
      Which[MemberQ[wrappedcells, #2],
        AppendTo[ls, SetPrecision[vpt - celltransvecAssoc[#2], 8] ],
        True, If[! MemberQ[ls, vpt], AppendTo[ls, vpt]]] &,
      ls, cellspartof]), {r1, r2}];

  newAdditions = Thread[(Range[Length@ls] + maxVnum) → ls],
  newAdditions = Thread[(Range[2] + maxVnum) → {r1, r2}]
  (* labels for new vertices *)
];
updatedLocalNetwork =
  Map[Partition[#, 2, 1, 1] &, Values[celltopologicalChanges], {2}];

 {$indToPtsAssoc, $ptsToIndAssoc, $cellVertexGrouping, $vertexToCell} =
  modifier[candidate, adjoiningCells, $indToPtsAssoc,
   $ptsToIndAssoc, $cellVertexGrouping, $vertexToCell,
   celltopologicalChanges, updatedLocalNetwork, newAdditions];

$faceListCoords =
  Map[Lookup[$indToPtsAssoc, #] &, $cellVertexGrouping, {2}];

$edges = Flatten[Map[Partition[#, 2, 1, 1] &, Map[
      Lookup[$indToPtsAssoc, #] &, Values[$cellVertexGrouping],
      {2}], {2}], 2] // DeleteDuplicatesBy[Sort];

With[{temp = Keys[$cellVertexGrouping]},
  $wrappedMat = AssociationThread[
    temp → Map[Lookup[$indToPtsAssoc, #] /. periodicRules &,
```

```
                 Lookup[$cellVertexGrouping, temp], {2}]
              ]];
           ])
         ]
        ]
      ]) &, selectTriangle];
   {$edges, $indToPtsAssoc,
    $ptsToIndAssoc, $cellVertexGrouping, $vertexToCell, $wrappedMat}
  ];
```

In[ ]:=

visualizing mesh

In[ ]:=
```
ClearAll[displayMesh];
Options[displayMesh] = Options[Graphics3D] ~ Join ~ {"opacity" → Opacity[1]};
displayMesh::"header" =
  "display the mesh of polyhedrons and colour by various properties;
colourmaps include:
    \"volume\",\"surfacearea\",\"height\",\"centroid\",\"faces\",\"surface/volume\",
    \"vertices\",\"edges\";
use None for displaying mesh without colouring";
displayMesh[indToPtsAssoc_, cellVertexG_, colourmap_ : "volume",
   opts : OptionsPattern[]] := Block[{mesh, col, plt, cellfaces, func},
   func = Function[x, ColorData["Rainbow"][x], Listable];
   cellfaces = Map[Lookup[indToPtsAssoc, #] &, cellVertexG, {2}];
   mesh = Values[Polyhedron@Flatten[triangulateToMesh@#, 1] & /@ cellfaces];
   plt = If[colourmap =!= None,
     col = func@Rescale@Switch[colourmap,
         "volume", Volume@mesh,
         "surfacearea" | "surface", SurfaceArea@mesh,
         "height", Values[Max[#[[All, All, 3]]] & /@ cellfaces],
         "centroid", (RegionCentroid /@ mesh)[[All, 3]],
         "faces", Values[Map[Length]@cellfaces],
         "surface/volume", (SurfaceArea@mesh) / (Volume@mesh),
         "vertices", Values[Length@*DeleteDuplicates@Flatten[#, 1] & /@ cellfaces],
         "edges", Values[(x ↦ Length@DeleteDuplicatesBy[Flatten[
                Partition[#, 2, 1, 1] & /@ x, 1], Sort]) /@ cellfaces]
        ];
      Thread[{col, mesh}],
     mesh
    ];
   Graphics3D[{OptionValue["opacity"], plt}, ImageSize → OptionValue[ImageSize]]
  ];
```

In[ ]:=
```
convertToPolyhed[table_, CVG_] :=
  (Polyhedron@Flatten[triangulateToMesh[#], 1] & /@ Map[Lookup[table, #] &, CVG, {2}]);
```

In[ ]:=
```
visualizeMesh[table_, CVG_] :=
  Graphics3D[Values@convertToPolyhed[table, CVG], ImageSize → 750];
```

main f(x)

In[ ]:=
```
$cellfaces = Map[Lookup[indToPtsAssoc, #] &, cellVertexGrouping, {2}];
$mesh = Values[Polyhedron@Flatten[triangulateFaces@#, 1] & /@ $cellfaces];
```

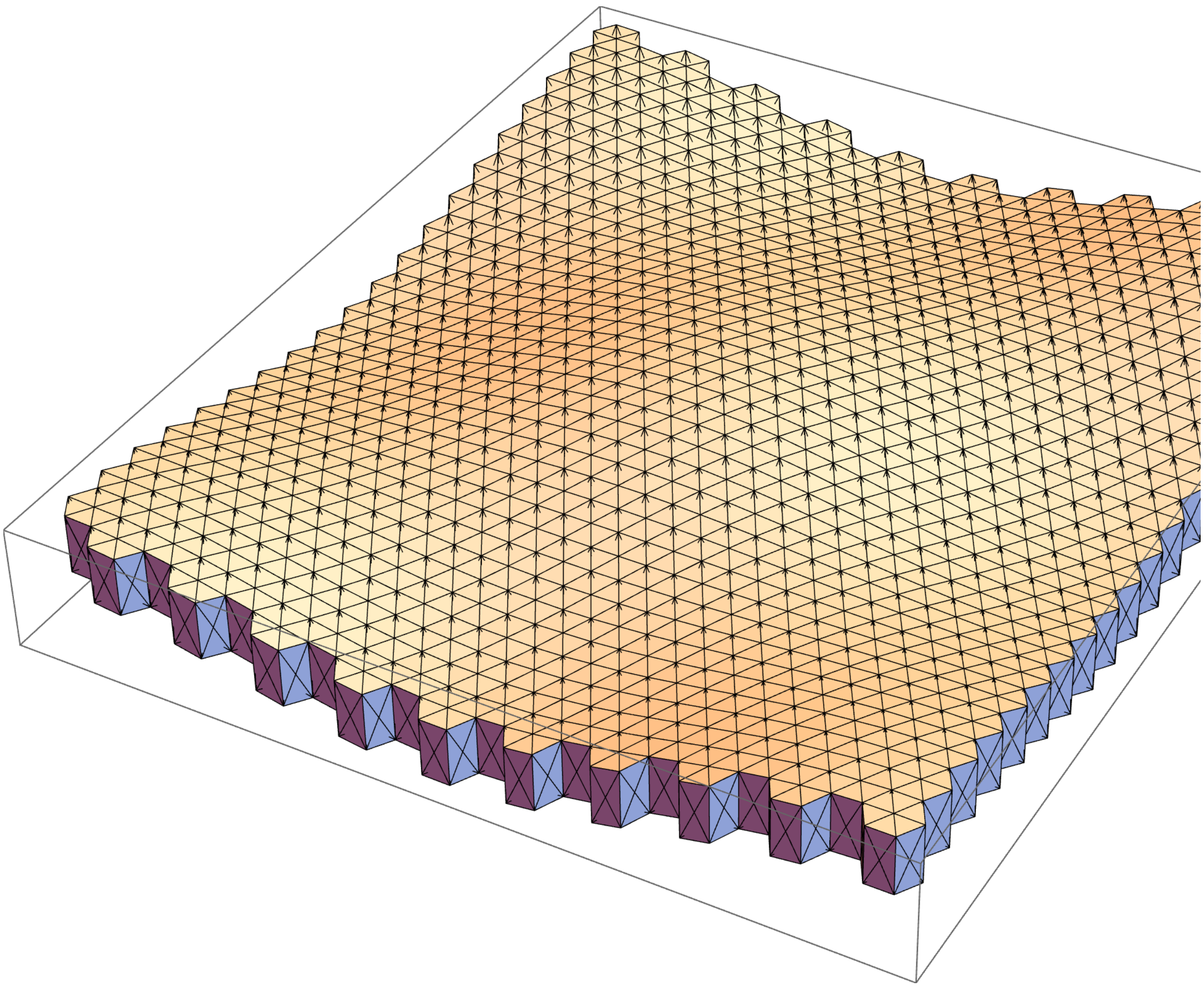
In[ ]:=
```
Mean[Volume@$mesh]
```

Out[ ]=
```
0.52611
```

1. instantiate geometry
2. seed growing cells in the tissue
3. initiate counter, and time-step = δt
4. main loop (? termination condition is fulfilled):
    - counter += 1
    - if Mod[counter, 10] is 0 :
        check for (I → Δ) & (Δ → I) transitions
    - perform *RK4* mesh integration
    - time += δt
5. visualize mesh

starting mesh

In[ ]:=
```
visualizeMesh[indToPtsAssoc, cellVertexGrouping]
```

Out[ ]=


test module (single time-step)

termination condition:

Abs[η (pts-coords @ t + 1 - pts-coords @ t)/δt] - ∇ at pts @ t < threshold

→ the condition should hold true for all pts

```
(* initialize time *)
```

In[ ]:=
```
time = 1 * δt;
```

In[•]:=
```
Clear@runSingleStep;
runSingleStep::Information = "test vertex model by running a single time step";
runSingleStep[ptsToIndAssoc_, indToPtsAssoc_, vertexToCell_, cellVertexGroup_] :=
  With[{ylim1 = yLim⟦1⟧,
    ylim2 = yLim⟦2⟧, xlim2 = xLim⟦2⟧},
   Block[{$ptsToIndAssoc = ptsToIndAssoc,
     $indToPtsAssoc = indToPtsAssoc, $vertexToCell = vertexToCell,
     $cellVertexGroup = cellVertexGroup, $wrappedMat,
     $wrappedMatTrim, $faceListCoords, $topo, vertKeys,
     cellKeys, boundarycells, bptpairs, outerptscloudTab,
     $indToPtsAssocOrig = indToPtsAssoc},
    cellKeys = Keys[$cellVertexGroup];
    vertKeys = Keys@$indToPtsAssoc;
    $faceListCoords = Map[Lookup[$indToPtsAssoc, #] &, $cellVertexGroup, {2}];
    $wrappedMat = With[{keys = Keys[$cellVertexGroup]},
      AssociationThread[keys → Map[Lookup[$indToPtsAssoc, #] /. periodicRules &,
         Lookup[$cellVertexGroup, keys], {2}]]
     ];
    boundarycells = outerCellsFn[$faceListCoords, $vertexToCell, $ptsToIndAssoc];
    $wrappedMatTrim = $wrappedMat~KeyTake~boundarycells;
    $topo = <|# → (getLocalTopology[$ptsToIndAssoc,
           $indToPtsAssoc, $vertexToCell, $cellVertexGroup,
           $wrappedMatTrim, $faceListCoords][$indToPtsAssoc[#]]) & /@ vertKeys|>;
    Echo["RK4 integration Started"];
    $indToPtsAssoc = RK4Integrator[$indToPtsAssoc,
      $topo, $cellVertexGroup, $vertexToCell, $ptsToIndAssoc];
    $ptsToIndAssoc = AssociationMap[Reverse, $indToPtsAssoc];
    Echo["Integration Done"];
    $indToPtsAssoc
   ]
  ];
```

In[•]:=
```
ClearSystemCache[];
```

In[•]:=
```
resSingleStep = runSingleStep[ptsToIndAssoc,
    indToPtsAssoc, vertexToCell, cellVertexGrouping]; // AbsoluteTiming
```

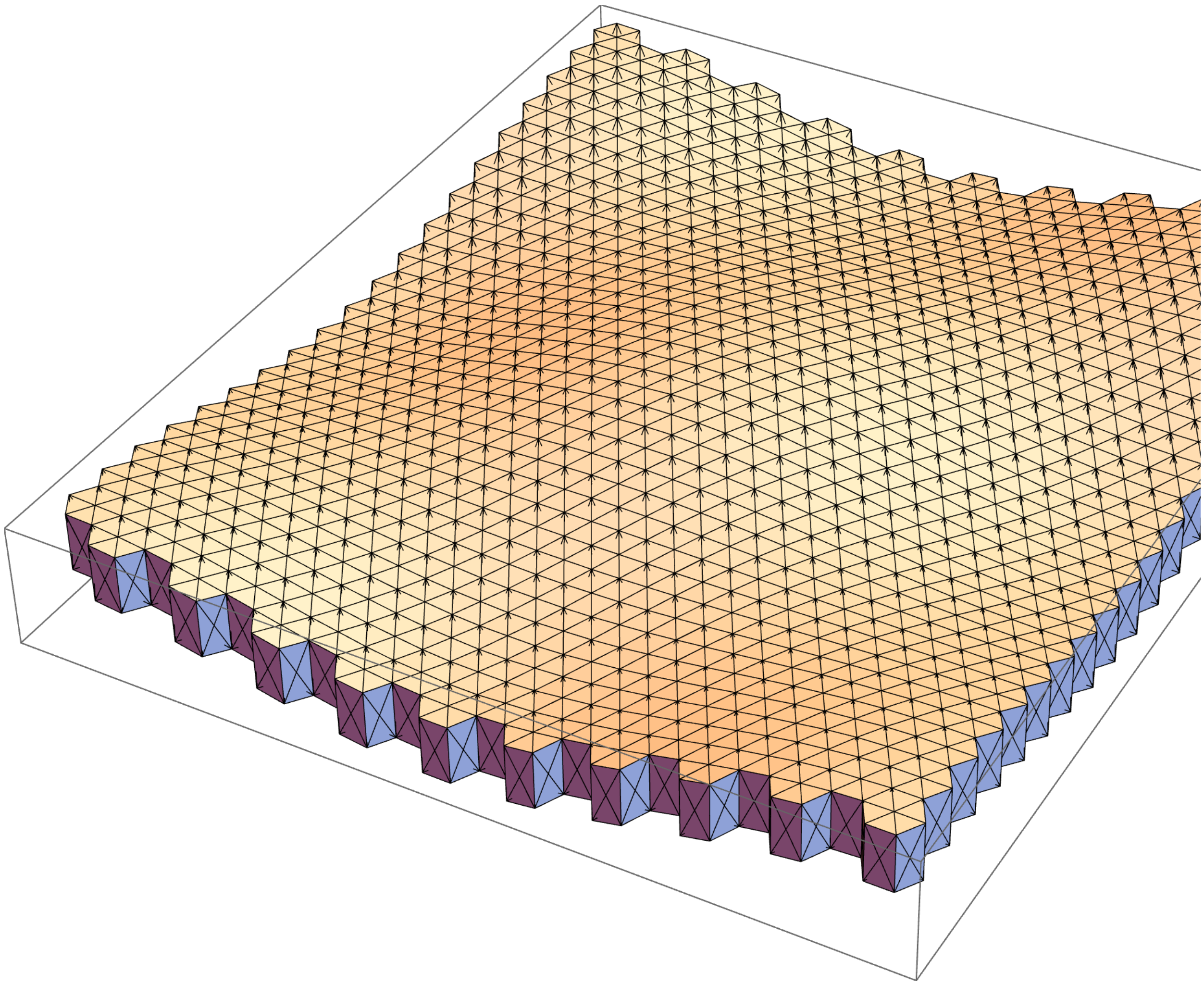
» RK4 integration Started

» Integration Done

Out[•]=
```
{8.10642, Null}
```

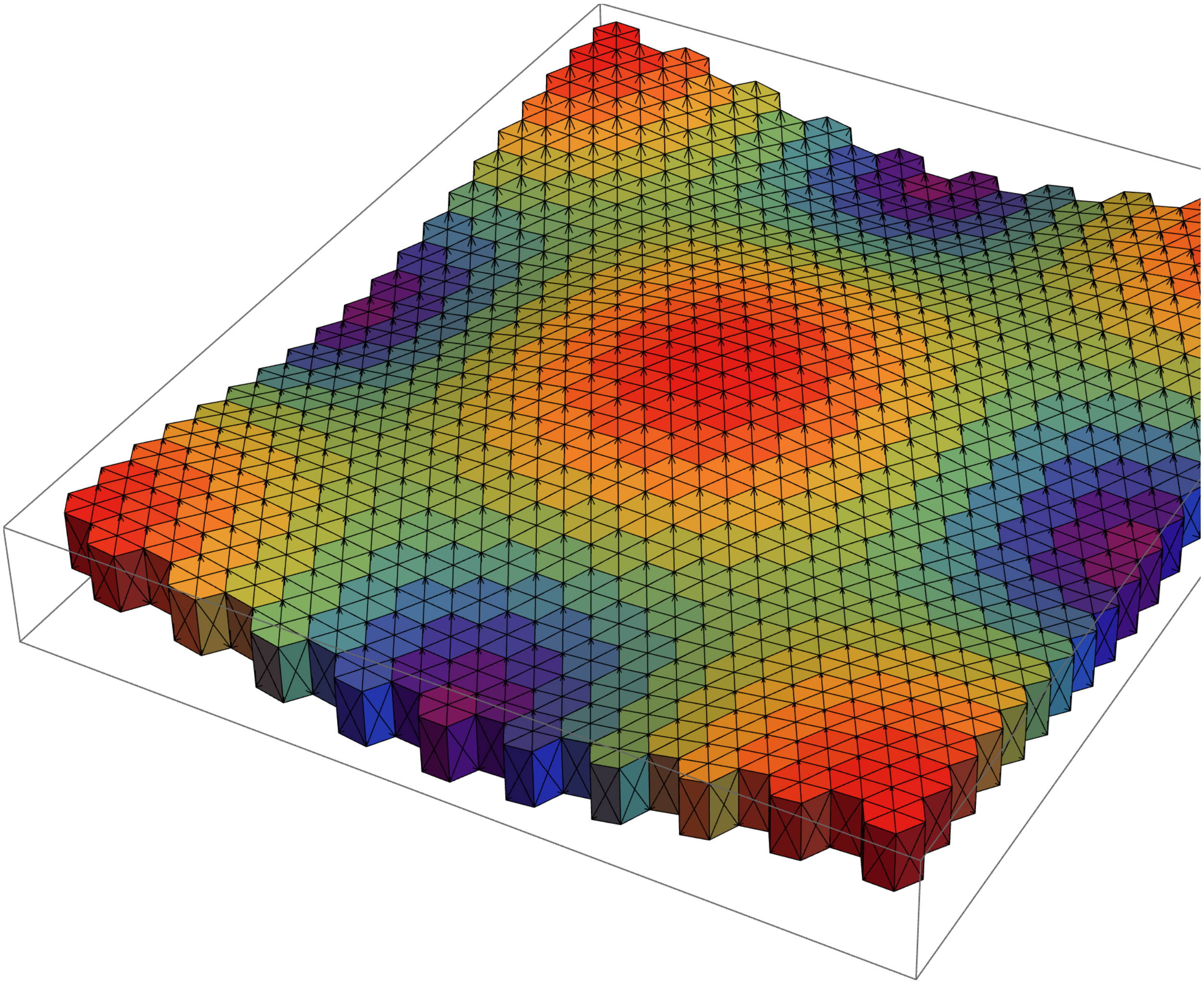
In[ ]:= **resSingleStep ~ visualizeMesh ~ cellVertexGrouping**

Out[ ]=



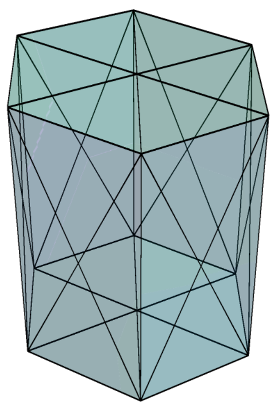
In[ ]:= **displayMesh[resSingleStep, cellVertexGrouping, "height", ImageSize → {750, Automatic}]**

Out[ ]=



In[ ]:=
```
Function[ind,
  With[{CVG = cellVertexGrouping[ind]},
   Show[Graphics3D[{Opacity[0.12], Green, (Polyhedron@Flatten[triangulateToMesh[#], 1] &@
         (Lookup[indToPtsAssoc, #] & /@ CVG))}],
    Graphics3D[{Opacity[0.12], Blue, (Polyhedron@Flatten[triangulateToMesh[#], 1] &@
         (Lookup[resSingleStep, #] & /@ CVG))}],
    ImageSize → Small, Boxed → False]
  ]
 ][1]
```

Out[ ]=



In[ ]:=
```
Clear@runModel;
runModel[ptsToIndAssoc_, indToPtsAssoc_, vertexToCell_, cellVertexGroup_] :=
  Block[{counter = 1, $indToPtsAssoc = indToPtsAssoc, $ptsToIndAssoc = ptsToIndAssoc,
    $cellVertexGroup = cellVertexGroup, $vertexToCell = vertexToCell,
    $wrappedMat, $faceListCoords, cellIds = Keys@cellVertexGroup,
    vertKeys, topo, boundarycells, $edges, $wrappedMatBound,
    $indToPtsAssocOrig = indToPtsAssoc, outerptscloudTab, bptpairs,
    endc = 30},
   time = counter * δt;
   Echo[time, "time: "];

   While[counter ≤ endc,
    Echo[counter, "counter: "];
    $faceListCoords = Map[Lookup[$indToPtsAssoc, #] &, $cellVertexGroup, {2}];
    $wrappedMat =
     AssociationThread[cellIds → Map[Lookup[$indToPtsAssoc, #] /. periodicRules &,
        Lookup[$cellVertexGroup, cellIds], {2}]];

    PrintTemporary[" ------ construct local topology ------ "];
    vertKeys = Keys@$indToPtsAssoc;
    cellIds = Keys@$cellVertexGroup;
    boundarycells = outerCellsFn[$faceListCoords, $vertexToCell, $ptsToIndAssoc];
    (*Print@boundarycells;*)
    $wrappedMatBound = $wrappedMat~KeyTake~boundarycells;
    topo = <|# → (getLocalTopology[$ptsToIndAssoc,
            $indToPtsAssoc, $vertexToCell, $cellVertexGroup,
            $wrappedMatBound, $faceListCoords][$indToPtsAssoc[#]]) & /@ vertKeys|>;
    (*Print[Values@Map[Length@*First,topo]//Counts];*)
    (*Print[
      Union@Values[Length@DeleteDuplicates@Flatten[Values[First@#],2]&/@topo]];*)
    PrintTemporary[" ------ Integrate mesh (RK4) ------ "];
    $indToPtsAssoc = RK4Integrator[$indToPtsAssoc,
      topo, $cellVertexGroup, $vertexToCell, $ptsToIndAssoc];
    $ptsToIndAssoc = AssociationMap[Reverse, $indToPtsAssoc];
    (*DumpSave["C:\\Users\\aliha\\Desktop\\vertmodelres\\datasave_"<>
       ToString[counter]<>"_"<>ToString[time]<>".mx",
      {$indToPtsAssoc,$ptsToIndAssoc,$cellVertexGroup,$vertexToCell}];*)
    time += δt; counter += 1;
    PrintTemporary["< update time > : " <> ToString[time]];
   ];
   Print[" ------ iterations ended successfully ------ "];
   {$ptsToIndAssoc, $indToPtsAssoc, $vertexToCell, $cellVertexGroup}
  ];
```

In[ ]:=
```
{res1, res2, res3, res4} = runModel[ptsToIndAssoc,
    indToPtsAssoc, vertexToCell, cellVertexGrouping]; // AbsoluteTiming
```

» time: 0.005

» counter: 1

» counter: 2

» counter: 3

» counter: 4

» counter: 5

» counter: 6

» counter: 7

» counter: 8

» counter: 9

» counter: 10

» counter: 11

» counter: 12

» counter: 13

» counter: 14

» counter: 15

» counter: 16

» counter: 17

» counter: 18

» counter: 19

» counter: 20

» counter: 21

» counter: 22

» counter: 23

» counter: 24

» counter: 25

» counter: 26

Missing[NotFound]

Missing[NotFound]

» counter: 27

» counter: 28

» counter: 29

» counter: 30

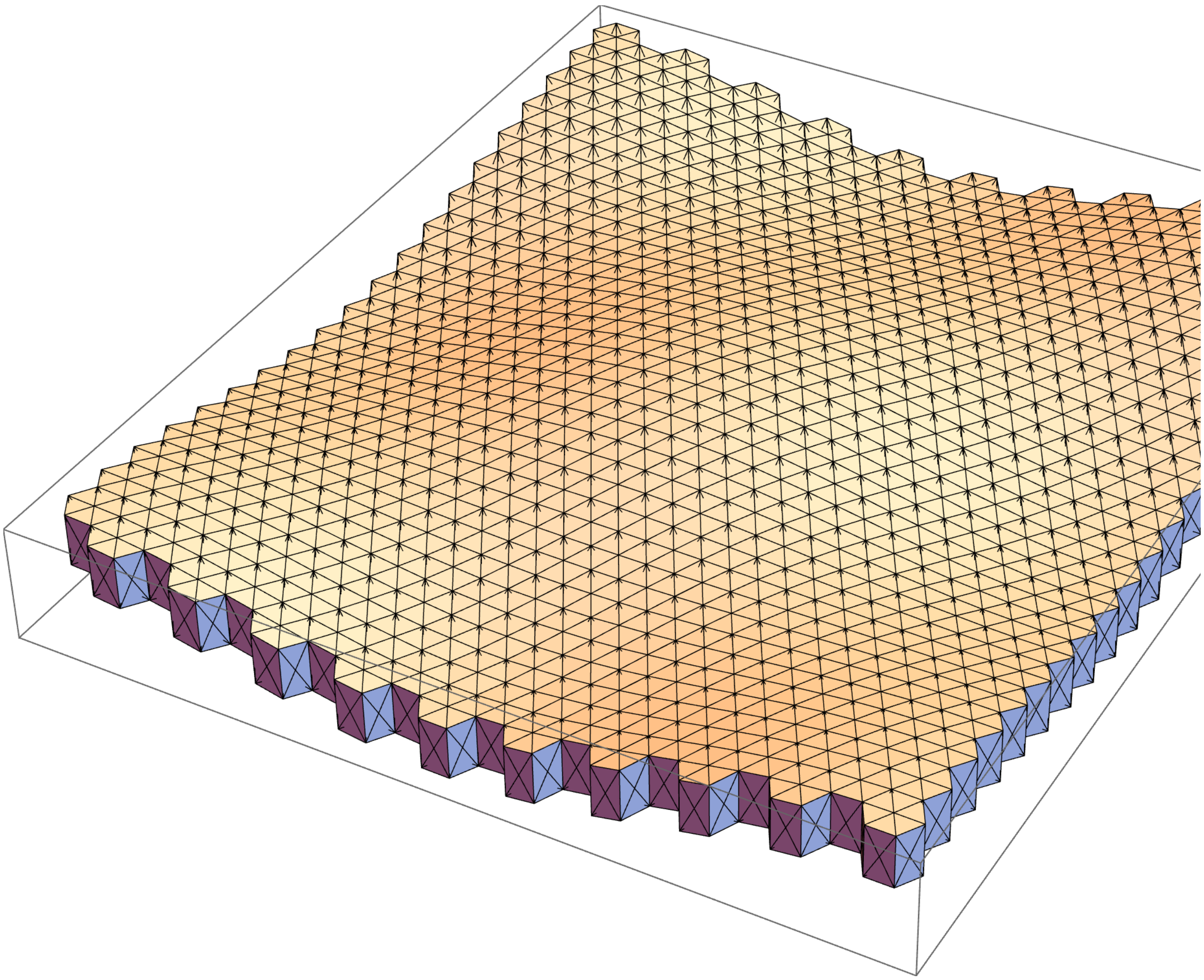
Missing[NotFound]

------ iterations ended successfully ------

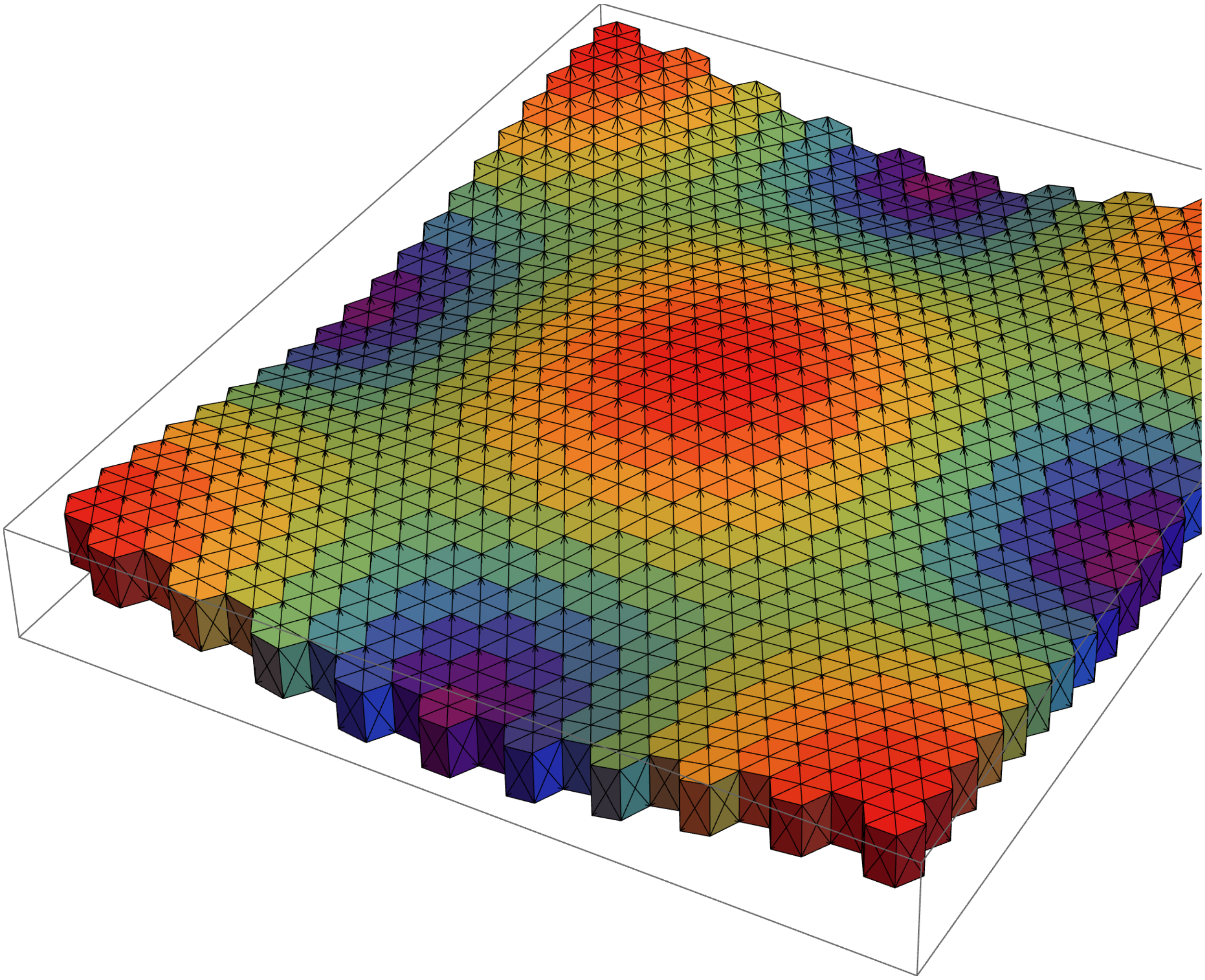
Out[•]= {283.107, Null}

In[ ]:= **res2 ~ visualizeMesh ~ res4**

Out[ ]=

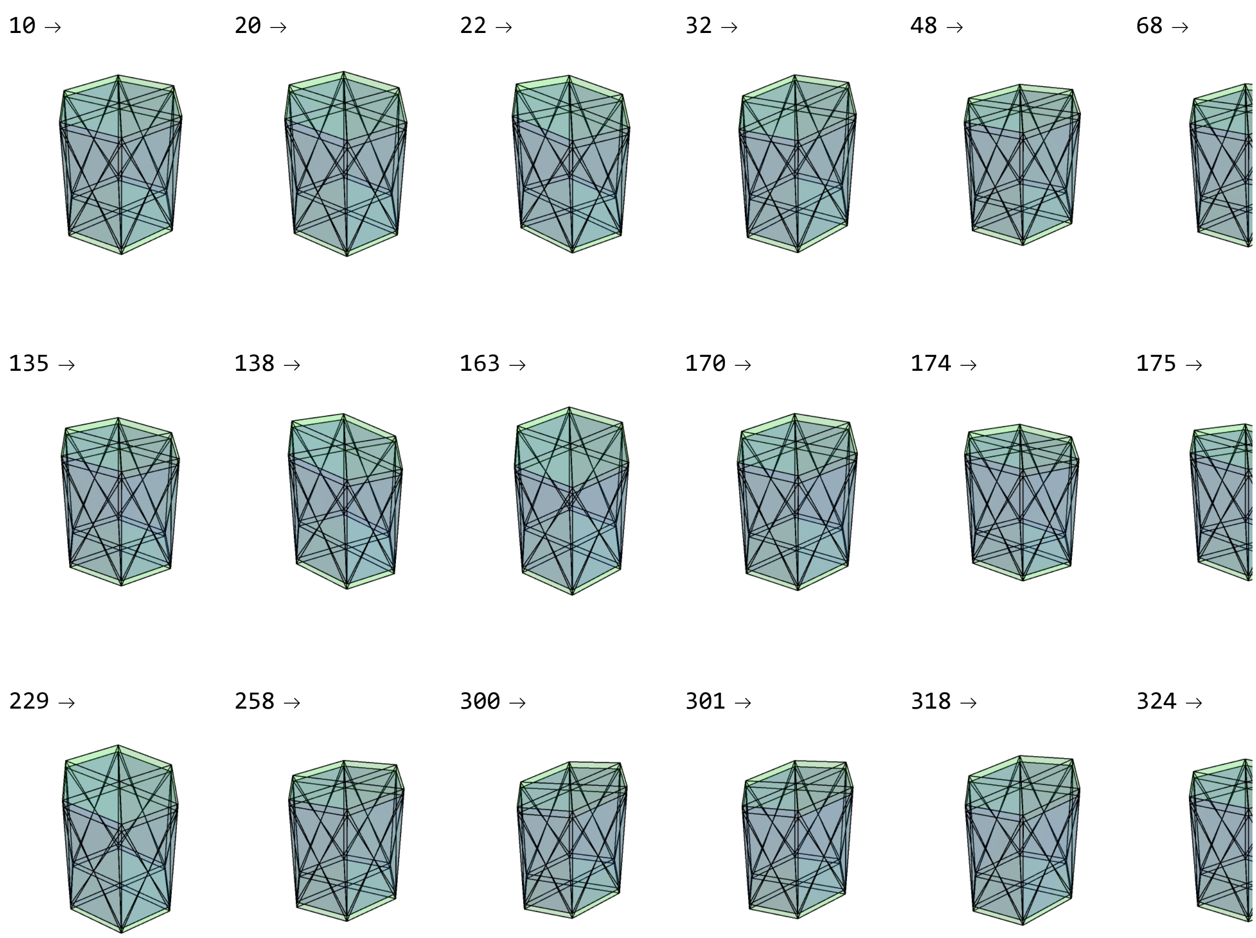


In[ ]:=
```
displayMesh[res2, cellVertexGrouping, "height", ImageSize → {750, Automatic}]
```

Out[ ]=


In[∘]:=
```
SeedRandom[1];
Grid[
 Partition[
  Function[ind,
    ind → With[{CVG = cellVertexGrouping[ind]},
      Show[Graphics3D[{Opacity[0.12], Blue,
          (Polyhedron@Flatten[triangulateToMesh[#], 1] &@ (Lookup[res2, #] & /@ CVG))}],
       Graphics3D[{Opacity[0.12], Green, (Polyhedron@Flatten[triangulateToMesh[#], 1] &@
            (Lookup[indToPtsAssoc, #] & /@ CVG))}],
       ImageSize → Tiny, Boxed → False]
     ]
   ] /@ Sort@RandomSample[Range[400], 30], 10]
]
```

Out[∘]=



In[∘]:=
```
$cellfaces = Map[Lookup[res2, #] &, cellVertexGrouping, {2}];
$mesh = Values[Polyhedron@Flatten[triangulateFaces@#, 1] & /@ $cellfaces];
```

In[∘]:=
```
Mean[Volume@$mesh]
```

Out[∘]= 0.470169

In[ ]:=
```
Sort@growingcellIndices
```

Out[ ]=
```
{7, 12, 18, 21, 28, 39, 42, 52, 90, 91, 96, 115, 125, 127,
 163, 204, 233, 249, 251, 266, 272, 282, 286, 289, 298, 300, 360, 386}
```