

Detecting nematic defects

```
In[1]:= ClearAll["Global`*"];
```

Code

```
In[2]:= Clear[imageOrientationFn];
imageOrientationFn[image_, rad_] := Block[
  {gy, gx, kernel1 = {1, 0}, kernel2 = {0, 1}, orientationParallel, orientationPerp},
  gy = GaussianFilter[image, rad, kernel1];
  gx = GaussianFilter[image, rad, kernel2];
  orientationParallel = 
$$\frac{1}{2} \text{ArcTan}[(gy * gy) - (gx * gx), 2 (gx * gy)];$$

  orientationPerp = ArcTan[ $\text{Sin}[orientationParallel]$ ,  $-\text{Cos}[orientationParallel]$ ];
  {orientationParallel, orientationPerp}
];
```

```
In[4]:= SetAttributes[makeVecs, HoldAll];
makeVecs[vals_, vecs_, s_, rQ_] :=
  With[{n = Length[vals]}, If[TrueQ[rQ], Do[Switch[Sign[Im[vals[[k]]]], 0, Null, 1,
    vecs[[k]] += s I vecs[[k + 1]], -1, vecs[[k]] = Conjugate[vecs[[k - 1]]]], {k, n}]];
Options[getEigensystem] = {Mode → Automatic};
getEigensystem[mat_?SquareMatrixQ, opts : OptionsPattern[]] :=
  Module[{m = mat, chk, ei, ev, lm, lv, n, rm, rQ, rv},
    n = Length[mat];
    Switch[OptionValue[Mode],
      Right | Automatic,
      {lm, rm} = {"N", "V"},
      Left, {lm, rm} = {"V", "N"},
      All, {lm, rm} = {"V", "V"},
      _, {lm, rm} = {"N", "V"}];
    LinearAlgebra`LAPACK`GEEV[lm, rm, m, ev, ei, lv, rv, chk, rQ];
    If[! TrueQ[chk],
      Message[getEigensystem::eivec0];
      Return[$Failed, Module]
    ];
    If[rQ, ev += I ei];
    Switch[OptionValue[Mode], Right | Automatic, rv = ConjugateTranspose[rv];
      makeVecs[ev, rv, 1, rQ]; {ev, rv}, Left, lv = ConjugateTranspose[lv];
      makeVecs[ev, lv, -1, rQ];
      {ev, lv}, All, {lv, rv} = ConjugateTranspose /@ {lv, rv};
      makeVecs[ev, rv, 1, rQ]; makeVecs[ev, lv, -1, rQ];
      {ev, rv, lv}, _, rv = ConjugateTranspose[rv];
      makeVecs[ev, rv, 1, rQ]; {ev, rv}]
  ];

```

```
In[8]:= winNumberFn[{dimx_, dimy_}, winsize_, overlap_] :=
  {Floor[(dimx - overlap)/(winsize - overlap)], Floor[(dimy - overlap)/(winsize - overlap)]};
```

```
In[9]:= ClearAll[discretizeFn];
discretizeFn[data_, winsize_, overlap_] := Block[{Nx, Ny, maxY, maxX, lsX, lsY},
  {maxY, maxX} = If[Length[#] == 2, #, Most@#] &@Dimensions[data];
  {Nx, Ny} = winNumberFn[{maxX, maxY}, winsize, overlap];
  lsX = Range[1, Nx] * winsize - Range[0, Nx - 1] * overlap - winsize/2;
  lsY = Range[1, Ny] * winsize - Range[0, Ny - 1] * overlap - winsize/2;
  {lsX, lsY}
];
```

```
In[11]:= ClearAll[dataPartFn];
dataPartFn[imagedata_, winsize_, overlap_] :=
  Block[{lsX, lsY, minx, miny, part, maxY, maxX},
    {lsX, lsY} = discretizeFn[imagedata, winsize, overlap];
    {maxY, maxX} = Dimensions[imagedata];

    part = Table[
      minx = Max[Floor[lsX[[i]] -  $\frac{\text{winsize}}{2}$ ], 1];
      miny = Max[Floor[lsY[[j]] -  $\frac{\text{winsize}}{2}$ ], 1];
      {
        {N@Mean@{minx, Floor[lsX[[i]] +  $\frac{\text{winsize}}{2}$ ]},,
         maxY - N@Mean@{miny, Floor[lsY[[j]] +  $\frac{\text{winsize}}{2}$ ]}}},
        imagedata[[miny ;; Floor[lsY[[j]] +  $\frac{\text{winsize}}{2}$ ], minx ;; Floor[lsX[[i]] +  $\frac{\text{winsize}}{2}$ ]]];
      }, {j, Ny}, {i, Nx}];
    Flatten[part, 1]^T
  ];

```

```
In[13]:= directorFieldFn[imageData_, winSize_, emptyCounts_] :=
  Block[{imgBoxData, zeroCount, θ, Γ, Λ, Π, Q, αβ, eigvals, eigvecs},
    ParallelTable[
      imgBoxData = Flatten[part];
      zeroCount = Count[imgBoxData, 0.];
      θ = imgBoxData /. 0. → Nothing;
      If[N[zeroCount / winSize^2] 100 ≤ emptyCounts,
        Length[θ]
        Qαβ = Sum[Γ = θ[[p]];
          {Λ, Π} = N[{Cos[Γ], Sin[Γ]}];
          3/2 (Λ^2 Λ Π) - 1/2 (1 0);
          2 (Λ Π Π^2)];
        If[Qαβ != 0,
          {eigvals, eigvecs} = Eigensystem[Qαβ / Length[θ]];
          First@Extract[eigvecs, Position[#, Max@#] &[Abs@eigvals]]
          (*First@Extract[eigvecs,Position[eigvals,Max@eigvals]]*)
          (*If[Abs[eigvals[[1]]] ≥ Abs[eigvals[[2]]], director = eigvecs[[1]]];
          If[eigvals[[2]] ≥ eigvals[[1]], director = eigvecs[[2]]];
          director*),
          Null],
          Null], {part, imageData}] /. Null → {Null, Null}
    ]
  ]
```

```
In[14]:= ClearAll[fnComp, JFn];
(*JFn[OrderlessPatternSequence[{Null, Null}, {Null, Null}] |
   OrderlessPatternSequence[{__Real}, {Null, Null}]] := None;*)
JFn[{Null, Null}, {Null, Null}] := None;
JFn[{__Real}, {Null, Null}] := None;
JFn[{Null, Null}, {__Real}] := None;

Block[{v1, v2, m, ang},
  fnComp = Compile[{{vec1, _Real, 1}, {vec2, _Real, 1}},
    v1 = vec1; v2 = vec2;
    ang = ArcTan[v1.v2, Abs[Det[{v1, v2}]]];
    If[ang > N[ $\frac{\pi}{2}$ ], v2 *= -1];
    m = Det[{v1, v2}];
    ang = Sign[m] ArcTan[v1.v2, Abs[m]],
    RuntimeOptions → "Speed", CompilationTarget → "C",
    CompilationOptions → {"ExpressionOptimization" → True}
  ]
]
]

JFn[x : {__Real} ..] := fnComp[x];

meshgrid[x_List, y_List] :=
{ConstantArray[x, Length[x]], Transpose@ConstantArray[y, Length[y]]};

If[$KernelCount == 0, LaunchKernels[]]
```

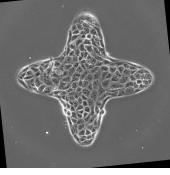
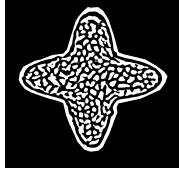
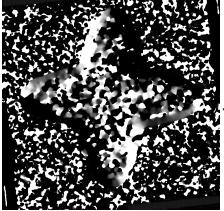
Out[18]=

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

Out[21]=

{KernelObject[Local KernelID: 1], KernelObject[Local KernelID: 2],
 KernelObject[Local KernelID: 3], KernelObject[Local KernelID: 4],
 KernelObject[Local KernelID: 5], KernelObject[Local KernelID: 6]}

Inputs

```
In[22]:= image = ; mask = ; orientationparallel = ;
```

```
In[23]:= (*image=ImageTrim[image,{\{1,52\},\{960,930\}}];
mask=ImageTrim[mask,{\{1,52\},\{960,930\}}];
orientationparallel=ImageTrim[orientationparallel,{\{1,52\},\{960,930\}}];*)

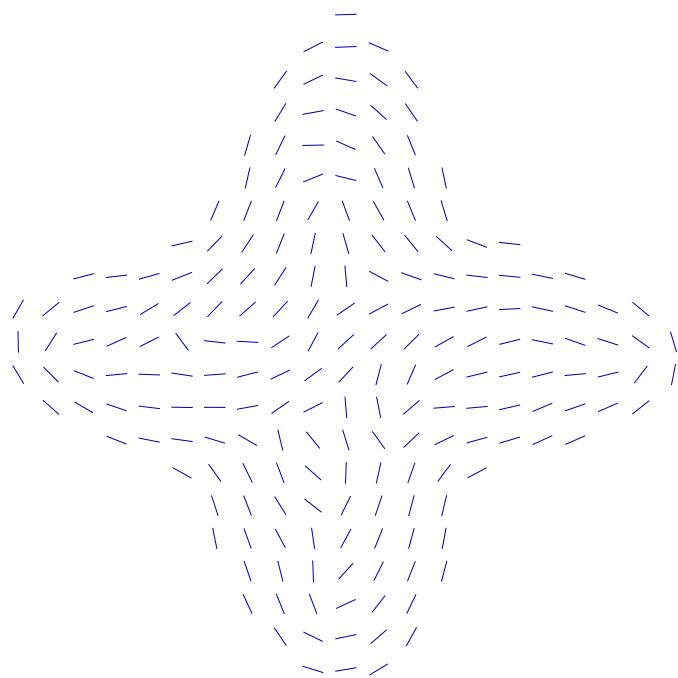
In[24]:= winsize = 100;
overlap = 60;
emptyCounts = 80;
colAssoc = <|0 → ▒,  $\frac{1}{2} \rightarrow \blacksquare$ ,  $-\frac{1}{2} \rightarrow \square$ , -1 → □, 1 → □|>;
```

Field Directors

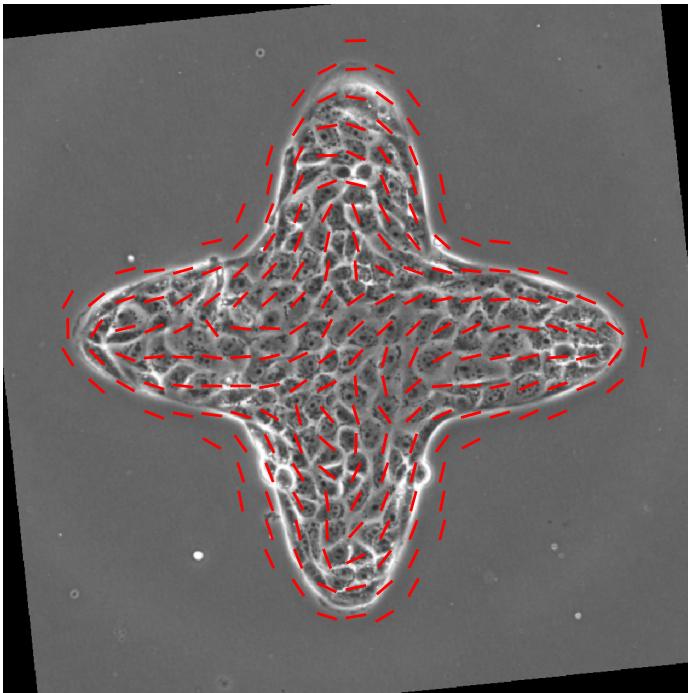
```
In[28]:= {dimx, dimy} = ImageDimensions[image]; (*{dimy,dimx}=Dimension[ImageData@image]*)
{Nx, Ny} = winNumberFn[{dimx, dimy}, winsize, overlap]; (*Nx are discretization in x-
axis or kind of columns and Ny are discretizations in y-axis or kind of rows*)
{midPtsWins, imagedata} =
  dataPartFn[ImageData[orientationparallel * mask], winsize, overlap];
directorfield = directorFieldFn[imagedata, winsize, emptyCounts];

In[32]:= directorScale =  $\frac{\text{winsize}}{8}$ ;
Graphics[{Darker@Blue, MapThread[
  If[#, == {0, 0}, Nothing, Line[{#2 + directorScale * #1, #2 - directorScale * #1}]] &,
  {directorfield /. Null → 0, midPtsWins}]}]
(*note: midPtsWins have been computed in image coordinate system here*)
HighlightImage[image, {Red, Thickness[0.004], MapThread[
  If[#, == {0., 0.}, Nothing, Line[{#2 + directorScale * #1, #2 - directorScale * #1}]] &,
  {directorfield /. Null → 0., midPtsWins}]}, ImageSize → Medium]
```

Out[33]=



Out[34]=



Winding Number

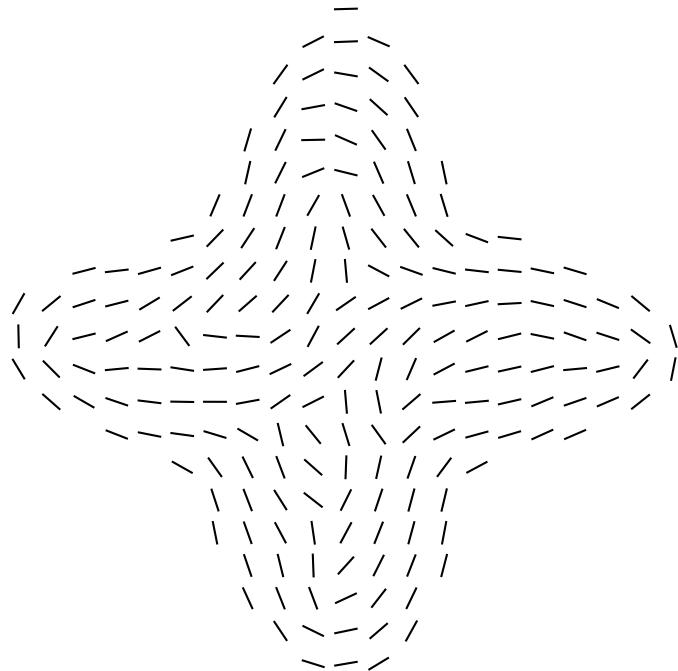
```
In[35]:= Partition[directorfield, Nx] === ArrayReshape[directorfield, {Ny, Nx, 2}]
parts = ArrayReshape[directorfield, {Ny, Nx, 2}] (*Partition[directorfield,Nx]*);
(*Nx represents the number of columns you need the directorfield to be divided into ..
  ofcourse appropriate rownumbers will be generated ..
  same as ArrayReshape[directorfield,{Ny,Nx,2}]*)
```

Out[35]=

True

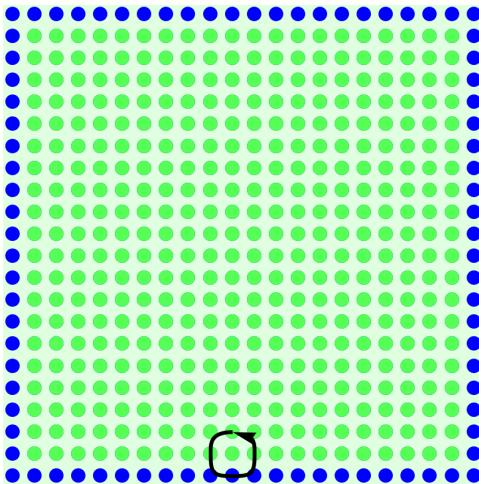
```
In[37]:= arr = Array[{\#\#} &, {Ny, Nx}];
assoc = <|Rule @@@ Flatten[{arr, parts}, {3, 2}]|>;
keys = Keys[assoc];
Graphics[ $\left\{ \text{Thickness}[0.003], \right.$ 
  KeyValueMap[If[#2 == {0, 0}, Nothing, Line[ $\left\{ \{\#1[[2]], Ny + 1 - \#1[[1]]\} + \frac{1}{3} \#2,$ 
     $\{\#1[[2]], Ny + 1 - \#1[[1]]\} - \frac{1}{3} \#2\} \right\}] \&, assoc /. Null \rightarrow 0] \left. \right\}, \text{ImageSize} \rightarrow \text{Medium}]$ 
```

Out[40]=



```
In[41]:= keystrunc = DeleteCases[keys, {1 | Ny, _} | {_, 1 | Nx}];
neighbours = {{0, 1}, {0, -1}, {-1, 0}, {1, 0}, {-1, 1}, {-1, -1}, {1, 1}, {1, -1}};
neighbourparts = {{neighbours[[1]], neighbours[[5]]}, {neighbours[[5]], neighbours[[3]]},
{neighbours[[3]], neighbours[[6]]}, {neighbours[[6]], neighbours[[2]]},
{neighbours[[2]], neighbours[[8]]}, {neighbours[[8]], neighbours[[4]]},
{neighbours[[4]], neighbours[[7]]}, {neighbours[[7]], neighbours[[1]]}};
keypairings = Map[keystrunc[[10]] + # &, neighbourparts, {2}];
Graphics[{{PointSize[0.03], Blue, Point@keys, Lighter@Green, Point@keystrunc},
Black, Thick, Arrowheads[Medium], Arrow[
BSplineCurve[DeleteDuplicates[Flatten[keypairings, 1]] ~Join~ {keypairings[[1, 1]]}]}}},
ImageSize → Small, Background → LightGreen] // Rasterize[#, "Image", ImageSize → 250] &
(*the plot is tilted ... horizontal is y and vertical is x*)
```

Out[45]=

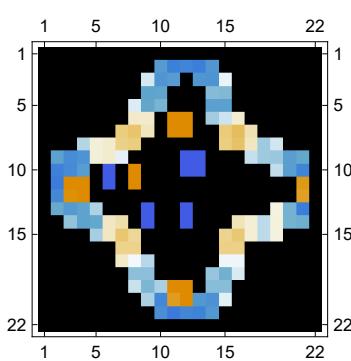


```
In[46]:= table = Table[
  keypairings = Map[i + # &, neighbourparts, {2}];
  Lookup[assoc, #] & /@ keypairings, {i, keystrunc}];

chargeArr = Rationalize[Chop@Total[Transpose[JFn @@ # & /@ table] /. None → 0] / (2 π)];

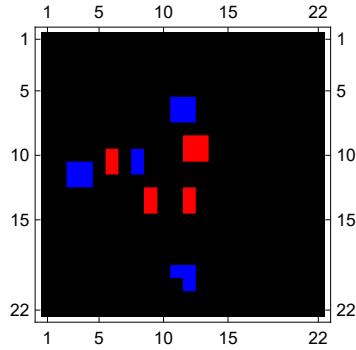
chargeArrTranspose = ArrayPad[Transpose@ArrayReshape[chargeArr, {Nx - 2, Ny - 2}], 1];
MatrixPlot[chargeArrTranspose, ColorRules → {0 → □}, ImageSize → Small]
```

Out[49]=



```
In[50]:= ε = 0.05;
chargeArrtranspose = Replace[chargeArrtranspose,
  {x_ /; N[1/2 - ε] ≤ x ≤ N[1/2 + ε] → 1/2, x_ /; N[-1/2 - ε] ≤ x ≤ N[-1/2 + ε] → -1/2}, {2}];
chargeArrtranspose = Replace[chargeArrtranspose, Except[1/2 | -1/2 | 1 | -1] → 0, {2}] ;
MatrixPlot[chargeArrtranspose,
 ColorRules → Thread[Keys@colAssoc → Values@colAssoc], ImageSize → Small]
```

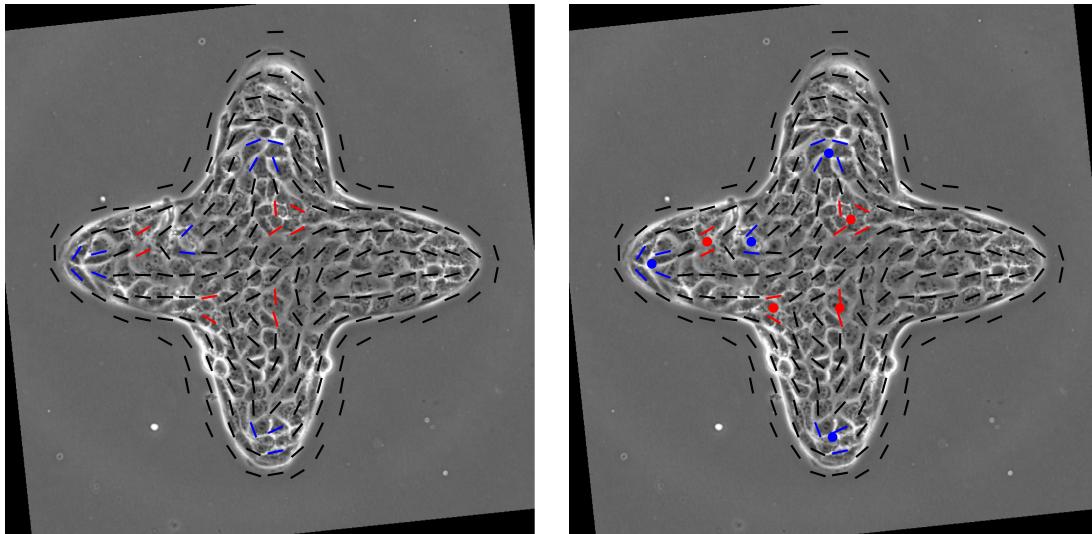
Out[53]=



```
In[54]:= arrmasks = SparseArray@
 MorphologicalComponents[ArrayComponents[chargeArrtranspose], CornerNeighbors → False];
posdefects =
 Mean@Extract[ArrayReshape[midPtsWins, Dimensions[chargeArrtranspose] ~Join~ {2}],
 Position[Normal@arrmasks, #]] & /@ Union@arrmasks["NonzeroValues"];
postype = Mean@Extract[chargeArrtranspose, Position[Normal@arrmasks, #]] & /@
 Union@arrmasks["NonzeroValues"];
```

```
In[57]:= directorfieldP = directorfield /. {Null, Null} → {0, 0};
GraphicsGrid[
{{{
  Rasterize[HighlightImage[image, MapThread[If[#1 != {0, 0},
    {colAssoc[#3], Thickness[0.004], Line[{#2 + winsize/8 #1, #2 - winsize/8 #1}]}] &,
    {directorfieldP, midPtsWins, Flatten[chargeArrtranspose]}}],
  ImageSize → Medium], "Image", ImageSize → 1024]
  ,
  Rasterize[HighlightImage[image,
  {MapThread[If[#1 != {0, 0},
    {colAssoc[#3], Thickness[0.004], Line[{#2 + winsize/8 #1, #2 - winsize/8 #1}]}] &,
    {directorfieldP, midPtsWins, Flatten[chargeArrtranspose]}}],
  MapThread[{colAssoc[#2], Point[#1]} &, {posdefects, postype}], ImageSize → Medium],
  "Image", ImageSize → 1024]
}
}]
]
```

Out[58]=



computing winding number from nematic angles

```
In[59]:= (*we can also compute the charge array using directly the
angles rather than the JFn function that deals with directors*)
```

```
In[60]:= directorToAngle[{Null, Null}] := None;
directorToAngle[director_] := ArcTan[director[[-1]] / director[[1]]];

In[62]:= nemAngles = Map[directorToAngle, parts, {2}] /. x_?NumericQ :> -x;

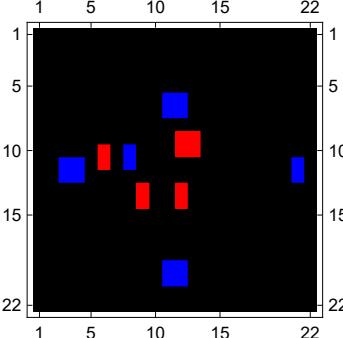
In[63]:= assoc2 = <|Rule @@@ Flatten[{arr, nemAngles}, {3, 2}]|>;
keys2 = Keys[assoc2];
keystrunc2 = DeleteCases[keys2, {1 | Ny, _} | {_, 1 | Nx}];

In[66]:= table2 = Table[
  keypairings = Map[(i + #) &, neighbourparts, {2}];
  assoc2[#] & /@ keypairings[[All, 1]], {i, keystrunc2}];

In[67]:= table2 = table2 /. x_? (Count[#, None] > 1 &) :> ConstantArray[None, 8];
(* the parameter 1 can be changed so that
charges are not calculated specifically with lots of NaNs*)

In[68]:= chargeArr2 =
  Map[Total] [Differences@*Reverse@* (Append[#, #[[1]]] &) /@ (table2 /. None :> 0) /.
  {x_ /; -π/2 ≤ x ≤ π/2 :> 0, x_ /; x < -π/2 :> π, x_ /; x > π/2 :> -π} ] / (2 π);

In[69]:= chargeArrtranspose2 = ArrayPad[Transpose@ArrayReshape[chargeArr2, {Nx - 2, Ny - 2}], 1];
MatrixPlot[chargeArrtranspose2,
ColorRules → Thread[Keys@colAssoc → Values@colAssoc], ImageSize → Small]

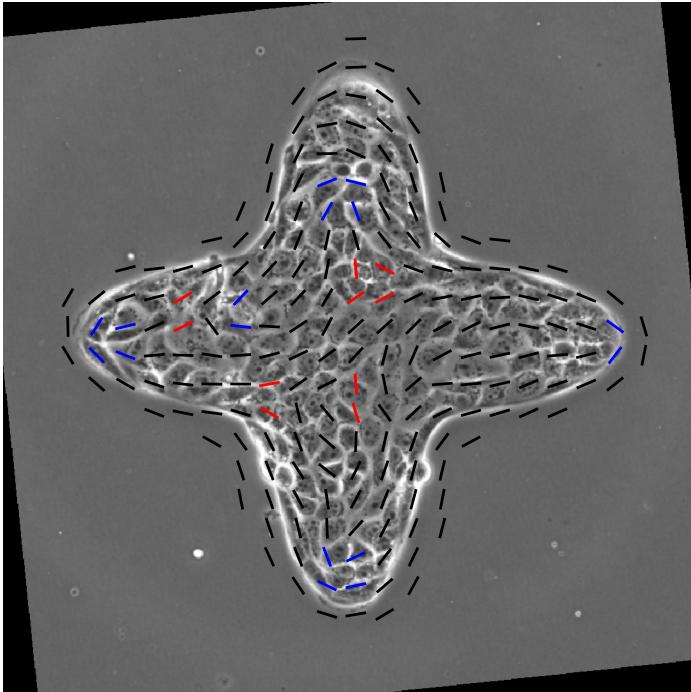
Out[70]=


```

```
In[71]:= arrmasks2 = SparseArray@MorphologicalComponents[
  ArrayComponents[chargeArrtranspose2], CornerNeighbors → False];
posdefects2 =
  Mean@Extract[ArrayReshape[midPtsWins, Dimensions[chargeArrtranspose2] ~Join~ {2}],
  Position[Normal@arrmasks2, #]] & /@ Union@arrmasks2["NonzeroValues"];
postype2 = Mean@Extract[chargeArrtranspose2, Position[Normal@arrmasks2, #]] & /@
  Union@arrmasks2["NonzeroValues"];
```

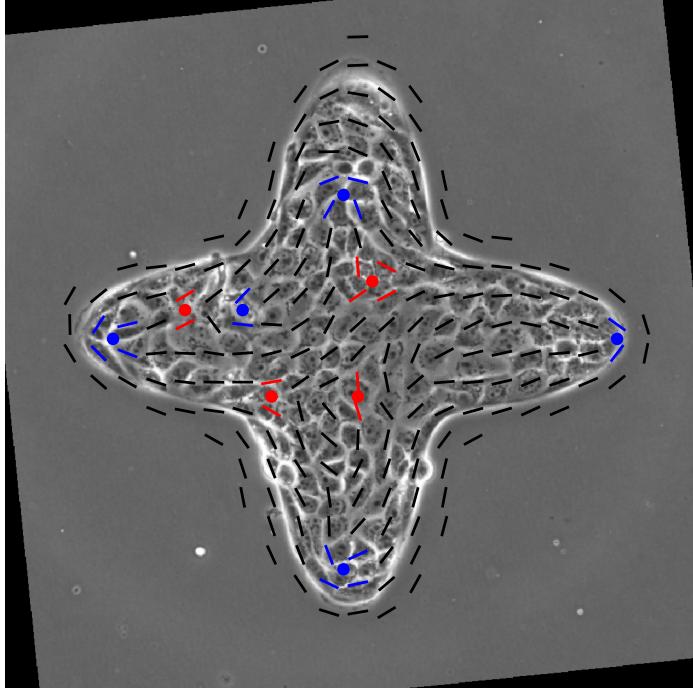
```
In[74]:= directorfieldP = directorfield /. {Null, Null} → {0, 0};  
HighlightImage[image, MapThread[If[#1 != {0, 0},  
{colAssoc[#3], Thickness[0.004], Line[{#2 + winsize/8 #1, #2 - winsize/8 #1}]}], &,  
{directorfieldP, midPtsWins, Flatten[chargeArrTranspose2]}], ImageSize → Medium]
```

Out[75]=



```
In[76]:= HighlightImage[image,
  {MapThread[If[#1 != {0, 0},
    {colAssoc[#3], Thickness[0.004], Line[{{#2 +  $\frac{\text{winSize}}{8}$  #1, #2 -  $\frac{\text{winSize}}{8}$  #1}}]}] &,
    {directorfieldP, midPtsWins, Flatten[chargeArrTranspose2]}],
  MapThread[{{colAssoc[#2], Point[#1]} &, {posdefects2, postype2}}], ImageSize -> Medium]
```

Out[76]=

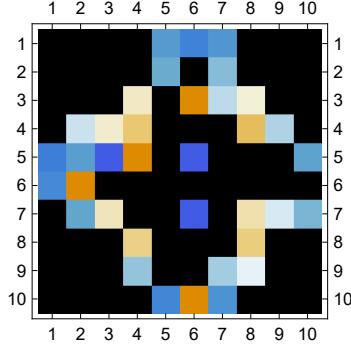


Winding number (subsampled)

```
In[77]:= Clear@dataPartFn2;
dataPartFn2[data_, {lsX_, lsY_}, winsize_, translation_, dimx_, dimy_] := Block[{Nx, Ny,
  maxXDir, maxYDir, rightX, leftX, rightY, leftY, overlap, part, midpt, indices},
  overlap = winsize - translation;
  {maxYDir, maxXDir} = Most@Dimensions[data];
  {Nx, Ny} = winNumberFn[{maxXDir, maxYDir}, winsize, overlap];
  Print[{Nx, Ny}];
  part = Table[
    rightX = i (winsize) - (i - 1) overlap;
    leftX = rightX - translation;
    rightY = j (winsize) - (j - 1) overlap;
    leftY = rightY - translation;
    midpt = Mean /@ {lsX[{leftX, rightX}], dimy - lsY[{leftY, rightY}]};
    indices = Mean /@ {{leftY, rightY}, {leftX, rightX}};
    {midpt, indices},
    {j, Ny}, {i, Nx}
  ];
  {{Nx, Ny}, part[[All, All, 1]], part[[All, All, -1]]}
];
In[79]:= {lsX, lsY} = discretizeFn[ImageData[orientationparallel], winsize, overlap];
{maxYDir, maxXDir} = Most@Dimensions[parts];
windowBox = 3;
translateBox = 2;
overlapWin = windowBox - translateBox;
In[84]:= {{Nx2, Ny2}, midpts, ls} =
  dataPartFn2[parts, {lsX, lsY}, windowBox, translateBox, dimx, dimy];
(*Nx2 are discretization in x-axis or kind of columns and Ny2 are discretizations in y-
 axis or kind of rows*)
ls = Flatten[ls, 1];
{10, 10}
```

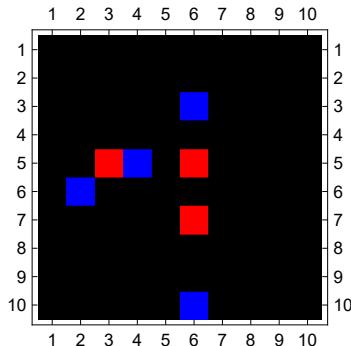
```
In[86]:= tablesubsampled = Table[
  keypairings = Map[i + # &, neighbourparts, {2}];
  Lookup[assoc, #] & /@ keypairings, {i, ls}];
chargeArrSampled =
  Rationalize[Chop@Total[Transpose[JFn @@@ # & /@ tablesubsampled] /. None -> 0] / (2 \pi)];
chargeArrtransposeSampled = ArrayReshape[chargeArrSampled, {Ny2, Nx2}];
(*Partition[chargeArrSampled,Nx2]*)
MatrixPlot[chargeArrtransposeSampled, ColorRules -> {0 -> □}, ImageSize -> Small]
```

Out[89]=

In[90]:= $\epsilon = 0.05$;

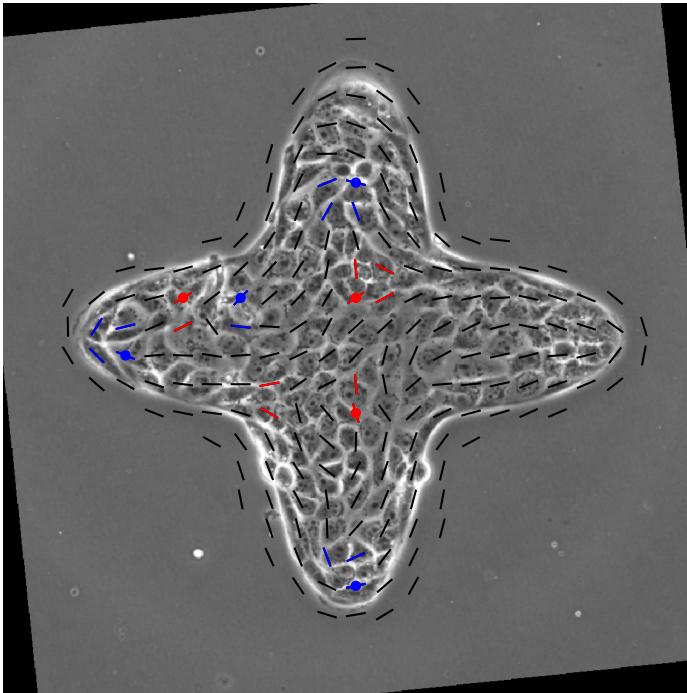
```
chargeArrtransposeSampled = Replace[chargeArrtransposeSampled,
  {x_ /; N[\frac{1}{2} - \epsilon] \leq x \leq N[\frac{1}{2} + \epsilon] \rightarrow \frac{1}{2}, x_ /; N[-\frac{1}{2} - \epsilon] \leq x \leq N[-\frac{1}{2} + \epsilon] \rightarrow -\frac{1}{2}], {2}];
chargeArrtransposeSampled =
  Replace[chargeArrtransposeSampled, Except[\frac{1}{2} | -\frac{1}{2} | 1 | -1] \rightarrow 0, {2}];
MatrixPlot[chargeArrtransposeSampled,
  ColorRules -> Thread[Keys@colAssoc -> Values@colAssoc], ImageSize -> Small]
```

Out[93]=



```
In[94]:= directorfieldP = directorfield /. {Null, Null} → {0, 0};
HighlightImage[image,
{Black, Thickness[0.003],
 MapThread[If[#1 === {0, 0}, Nothing, Line[{#2 + winsize/8 #1, #2 - winsize/8 #1}]] &,
 {directorfieldP, midPtsWins}],
 MapThread[If[#1 == {0, 0} || #3 == 0, Nothing,
 {colAssoc[#3], Line[{#2 + winsize/8 #1, #2 - winsize/8 #1}]}] &,
 {directorfieldP, midPtsWins, Flatten[chargeArrTranspose]}],
 PointSize[0.015], MapThread[If[#2 == 0, Nothing, {colAssoc[#2], Point[#1]}]] &,
 {Flatten[midpts, 1], Flatten[chargeArrTransposeSampled]}], ImageSize → Medium]
```

Out[95]=



computing winding number from nematic angles (subsampled)

```
In[96]:= (*we can also compute the charge array using directly the
angles rather than the JFn function that deals with directors*)

In[97]:= tableSubsampled2 = Table[keypairings = Map[i + # &, neighbourparts, {2}];
assoc2[#] & /@ keypairings[[All, 1]], {i, ls}];

In[98]:= tableSubsampled2 = tableSubsampled2 /. x_ ? (Count[#, None] > 1 &) :> ConstantArray[None, 8];
(* the parameter 1 can be changed so that
charges are not calculated specifically with lots of NaNs*)
```

```
In[99]:= chargeArrsubsampled2 = Map[Total] [
  Differences@*Reverse@* (Append[#, #[[1]]] &) /@ (tablesubsampled2 /. None -> 0) /.
  {x_ /; -π/2 ≤ x ≤ π/2 :> 0, x_ /; x < -π/2 :> π, x_ /; x > π/2 :> -π} ] / (2 π);

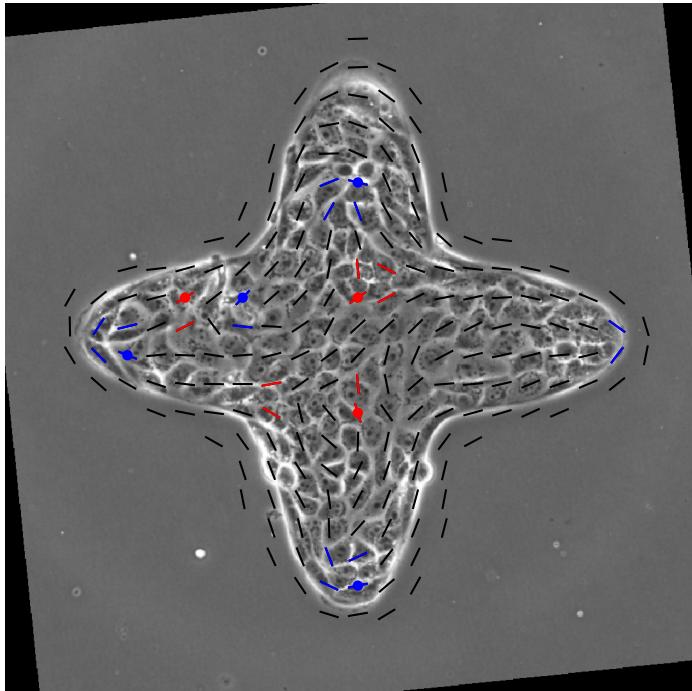
In[100]:= chargeArrsubsampledtranspose2 = ArrayReshape[chargeArrsubsampled2, {Ny2, Nx2}];
MatrixPlot[chargeArrsubsampledtranspose2,
 ColorRules -> Thread[Keys@colAssoc -> Values@colAssoc], ImageSize -> Small]

Out[101]=
```

The figure is a 10x10 grid plot. The x-axis and y-axis both range from 1 to 10. The plot area is black. There are several colored squares: a central horizontal row of alternating red and blue squares (approximately positions 3 to 7 on the x-axis), a red square at position (2, 2), a blue square at position (6, 2), a red square at position (2, 6), a blue square at position (6, 6), and a red square at position (6, 7). The plot has a white border.

```
In[102]:= directorfieldP = directorfield /. {Null, Null} → {0, 0};
HighlightImage[image,
{Black, Thickness[0.003],
 MapThread[If[#1 === {0, 0}, Nothing, Line[{#2 + winsize/8 #1, #2 - winsize/8 #1}]] &,
 {directorfieldP, midPtsWins}],
 MapThread[If[#1 == {0, 0} || #3 == 0, Nothing,
 {colAssoc[#3], Line[{#2 + winsize/8 #1, #2 - winsize/8 #1}]}] &,
 {directorfieldP, midPtsWins, Flatten[chargeArrtranspose2]}],
 PointSize[0.015], MapThread[If[#2 == 0, Nothing, {colAssoc[#2], Point[#1]}]] &,
 {Flatten[midpts, 1], Flatten[chargeArrsubsampledtranspose2]}]
}, ImageSize → Medium]
```

Out[103]=



Defect Annihilation

```
In[104]:= (*if two opposite defects are in close proximity they should annihilate*)
```

In[105]:=

```

ClearAll[annihateDefectFn];
annihateDefectFn[chargedarr_, midpts_, thresh_ : 80] :=
  Block[{defectlocAssoc, distmat, pos, loc, chArr = chargedarr, u, v, $u, Fn},
    Fn[$u_, t_, pts_] := (
      {u, v} = {defectlocAssoc[$u], defectlocAssoc[-$u]};
      If[Head[u] != Missing || Head[v] != Missing,
        distmat = DistanceMatrix[N[u], N[v]];
        While[Min[distmat] <= t && Length[distmat] > 1,
          pos = FirstPosition[distmat, Min@distmat];
          loc = Position[pts, Alternatives @@ {u[[pos[[1]]]], v[[pos[[2]]]]}];
          (chArr[[#\[If[1, 1, -1]]]] = 0) & /@ loc;
          u = Delete[u, pos[[1]]];
          v = Delete[v, pos[[2]]];
          distmat = DistanceMatrix[N[u], N[v]];
        ],
        Echo["defect pair +" <> ToString[$u] <> " & " <> ToString[-$u] <> " do not exist"];
      ]
    );
    defectlocAssoc =
      KeyDrop[GroupBy[Flatten[{chargedarr, midpts}, {2, 3}], First \[Rule] Last], 0];
    Fn[ $\frac{1}{2}$ , thresh, midpts];
    Fn[1, thresh, midpts];
    chArr
  ];

```

In[107]:=

(*remove defects within a certain threshold distance*)

In[108]:=

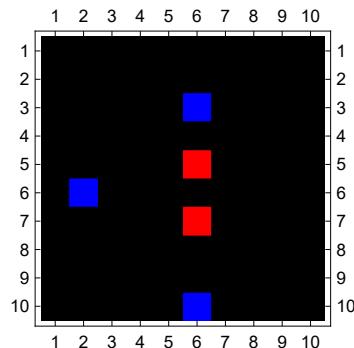
```

MatrixPlot[annihateDefectFn[chargeArrsubsampledtranspose2, midpts, 80],
  ColorRules \[Rule] Thread[Keys@colAssoc \[Rule] Values@colAssoc], ImageSize \[Rule] Small]

```

» defect pair +1 & -1 do not exist

Out[108]=



Defect Stability

In[114]:=

```

chargeStabilityFn[arrays_] := Block[{defectbreakdown,
  defectbreakdownFrameNum, chArr = arrays, defpos, temp, stableduration},
  defectbreakdown = Apply[Thread@*Rule] /@ Transpose[
    {Flatten@*Map[Union] @*Split /@ chArr, Map[Length] @*Split /@ chArr}, 1 < 2];
  defectbreakdownFrameNum =
    Map[Thread[Keys[#] > Accumulate@Values@#] &, defectbreakdown];
  temp = Position[defectbreakdown,  $\frac{1}{2} \rightarrow 1$ ] ~Join~ Position[defectbreakdown,  $-\frac{1}{2} \rightarrow 1$ ];
  (*the first indices represent position where unstable
   defects are located. defects that only appear in a single frame*)
  defpos = Thread[{temp[[All, 1]], Values@Extract[defectbreakdownFrameNum, temp]}];
  Do[chArr[[i[[1]], i[[1]]]] =
    Style[chArr[[i[[1]], i[[1]]]], Bold, Blue, Background > LightRed], {i, defpos}];

  temp = Position[defectbreakdown,  $\frac{1}{2} \rightarrow x_- /; x > 1$ ] ~
    Join~ Position[defectbreakdown,  $-\frac{1}{2} \rightarrow x_- /; x > 1$ ];
  (*position where stable defects are located*)
  stableduration = Cases[defectbreakdown, PatternSequence[ $\frac{1}{2} \rightarrow x_- /; x > 1$ ], {2}] ~Join~
    Cases[defectbreakdown, PatternSequence[ $-\frac{1}{2} \rightarrow x_- /; x > 1$ ], {2}] // Values;
  defpos = Thread[{temp[[All, 1]], Values@Extract[defectbreakdownFrameNum, temp]}];
  defpos = defpos ~Join~ Flatten[
    MapThread[Thread[{#[[1]], #[[2]] - Range[#[[2]] + 1]}] &, {defpos, stableduration}], 1];
  Do[chArr[[i[[1]], i[[1]]]] =
    Style[chArr[[i[[1]], i[[1]]]], Bold, Blue, Background > LightBlue], {i, defpos}];
  Transpose[chArr]
];

```

In[115]:=

```
Grid[chargeStabilityFn@madeupframes, Background -> White, Dividers -> {All, False}]
```

Out[115]=

In[116]:=

```
Grid[Prepend[Prepend[chargeStabilityFn@madeupframes,
  Style[#, Magenta] & /@ Range[Length@madeupframes]]^,
  Prepend[Style[ToExpression["t" <> ToString[##]], Magenta] & /@
    Range[Length[madeupframes^]],  $\frac{\text{pos}}{\text{time}}$ ]]]^, Dividers -> {{1, 2}, All}]
```

Out[116]=

$\frac{\text{pos}}{\text{time}}$	1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35
t1	0 0
t2	0 0 0 0 0 $\frac{1}{2}$ 0
t3	0 0 0 0 0 $\frac{1}{2}$ 0
t4	0 0 0 0 0 $\frac{1}{2}$ 0
t5	0 0

Defect Directionality (not important but a nice have to function)