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% Example_5_4.mlx
%
% This is Example 5.4 from the paper 'Laguerre tessellations and
% polycrystalline microstructures: A fast algorithm for generating grains
% of given volumes' by D.P. Bourne, P.J.J. Kok, S.M. Roper, W.D.T. Spanjer
% (Philosophical Magazine 100, 2677-2707, 2020).
%
% We generate a 3D periodic Laguerre diagram representing an idealised
% DP (dual phase) steel in which the two phases are arranged in layers.

clear

tic

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

% Specify whether the Laguerre diagram is periodic (periodic=true) or
% non-periodic (periodic=false)

periodic=true;

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% Define the geometry. We create a 3D periodic Laguerre diagram in a
% rectangular box with vertices (0,0,0), (L1,0,0), (0,L2,0), (0,0,L3),
% (L1,L2,0), (L1,0,L3), (0,L2,L3), (L1,L2,L3).

L1=2; % length of the box in the x-direction
L2=3; % length of the box in the y-direction
L3=2; % length of the box in the z-direction
bx=[L1,L2,L3];

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% Specify the desired volumes of the grains. These are stored in a column
% vector called target_vols.

NumLayers=3; % number of layers
nLayer=[1000;8000;1000]; % number of grains per layer
rLayer=[1;0.05;1]; % size ratio of the grains per layer

N=sum(nLayer); % total number of grains
target_vols=zeros(N,1);
for j=1:NumLayers
    target_vols(sum(nLayer(1:j-1))+1:sum(nLayer(1:j-1))+nLayer(j))=...
        rLayer(j);
end

% Normalise the volumes so that they add to the volume of the box
target_vols = target_vols*L1*L2*L3/sum(target_vols);

% Set the phase ID to correspond to the grain size.
% The large grains have phaseID=1, the small grains have phaseID=2.

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phaseID=ones(size(target_vols));
phaseID(nLayer(1)+1:nLayer(1)+nLayer(2))=2;

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% Choose the optimisation solver

solver='dampedNewton'; % damped Newton method (recommended)
% solver='fminunc'; % slower option

% Remark:
% In the paper 'Laguerre tessellations and polycrystalline microstructures:
% A fast algorithm for generating grains of given volumes' by D.P. Bourne,
% P.J.J. Kok, S.M. Roper, W.D.T. Spanjer (2020), we used the MATLAB solver
% fminunc. A faster option is to use the damped Newton method, as
% described in 'Geometric modelling of polycrystalline materials: Laguerre
% tessellations and periodic semi-discrete optimal transport' by
% D.P. Bourne, M. Pearce & S.M. Roper (2022).

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% Initialise the seed locations

% Choose the x- and y-coordinates of the initial seed locations randomly
x0=L1*rand(N,1);
y0=L2*rand(N,1);

% Define the z-coordinates of the initial seed locations by placing the
% seeds in layers
vLayer=zeros(NumLayers,1); % desired volume of grains per layer
for j=1:NumLayers
    vLayer(j)=...
        sum(target_vols(sum(nLayer(1:j-1))+1:sum(nLayer(1:j-1))+nLayer(j)));
end
tLayer=vLayer/L1/L2; % desired thickness of each layer
z0=zeros(N,1);
for j=1:NumLayers
    z0(sum(nLayer(1:j-1))+1:sum(nLayer(1:j-1))+nLayer(j))=...
        tLayer(j)*rand(nLayer(j),1)+sum(tLayer(1:j-1));
end

X0=[x0,y0,z0]; % initial location of the seeds

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

% Perform Algorithm 2 from the paper 'Laguerre tessellations and
% polycrystalline microstructures: A fast algorithm for
% generating grains of given volumes' by D.P. Bourne, P.J.J. Kok,
% S.M. Roper, W.D.T. Spanjer (Philosophical Magazine 100, 2677-2707, 2020).

% Set the parameters of the algorithm
numLloyd=20; % number of regularisation (Lloyd) iterations
tol=1; % percentage error tolerance for the volumes of the grains

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% Perform Algorithm 2
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[X,w,percent_error,actual_vols]=...  
    algorithm2(bx,X0,target_vols,periodic,tol,numLloyd,solver);
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Lloyd iteration:1
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Lloyd iteration:2
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Warning: With the w_0 specified, there is at least one zero-volume cell
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Warning: Switch to using w_0=0 for the initial guess for damped Newton
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Lloyd iteration:3
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Lloyd iteration:4
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Lloyd iteration:5
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Lloyd iteration:6
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Lloyd iteration:7
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Lloyd iteration:8
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Lloyd iteration:9
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Lloyd iteration:10
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Lloyd iteration:11
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Lloyd iteration:12
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Lloyd iteration:13
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Lloyd iteration:14
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Lloyd iteration:15
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Lloyd iteration:16
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Lloyd iteration:17
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Lloyd iteration:18
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Lloyd iteration:19
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Lloyd iteration:20
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% Output the difference (percentage error) between the actual volumes of  
% the grains and the target volumes
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disp(strcat('Maximum percentage error=',num2str(percent_error),'%'));
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Maximum percentage error=0.083157%
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toc
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Elapsed time is 78.775165 seconds.
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% Save the results in a txt file
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x=X(:,1);
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y=X(:,2);
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z=X(:,3);
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fileID = fopen('Weight_data_Example_5_4.txt','w');
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fprintf(fileID,'%06d %5.3f %5.3f %5.3f %u \r\n',length(x),L1,L2,L3,int8(periodic));
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for i=1:length(x)
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    fprintf(fileID,'%06d %-3.7e %-3.7e %-3.7e %-3.7e %3.1f\r\n',...  
        [i,w(i),x(i),y(i),z(i),phaseID(i)]);
```

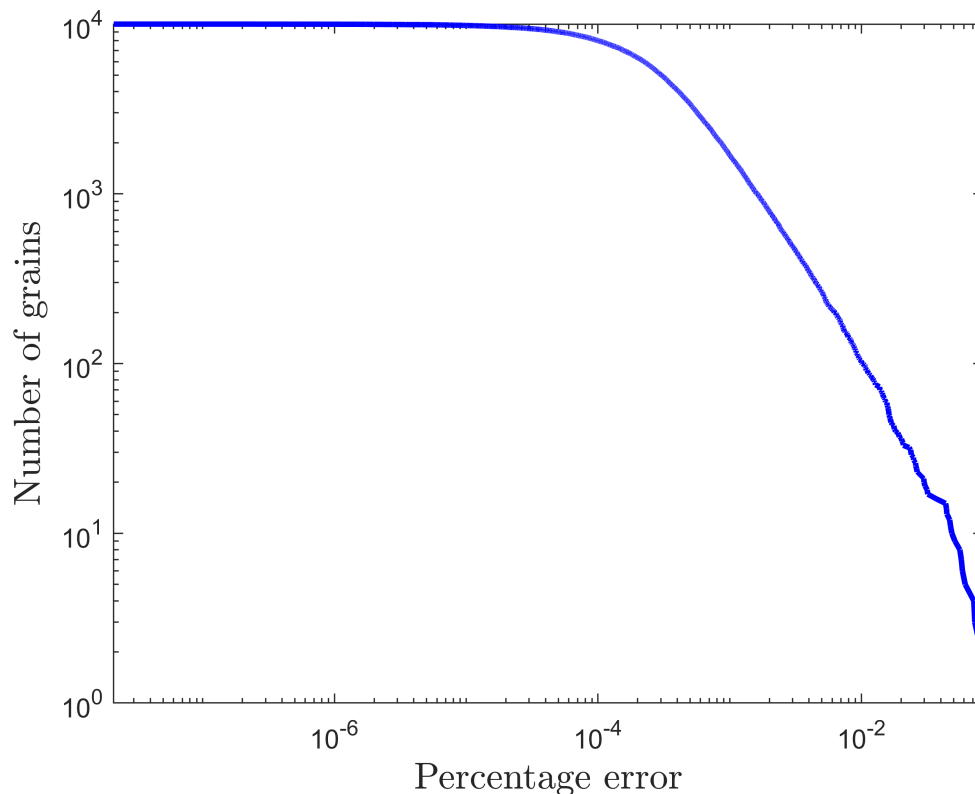
```
end
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fclose(fileID);
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% Plot the volume errors
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percentage_errors=100*abs(actual_vols-target_vols)./target_vols;
plotErrors(percentage_errors);
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drawnow
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% Plot the Laguerre tessellation
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% Compute the vertices, faces, neighbours (vfn) of the Laguerre diagram
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[~,~,~,vfn]=mexPDall(bx,X,w,periodic);
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% Compute which cells lie on the boundary of the box (no need to plot the
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% interior cells since they are not visible)
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[polys,cellids]=intersect_cells_on_boundary_periodic(bx,vfn);
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% Colour the grains according to their volume
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myc=generateGrainColours(actual_vols);
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```
% Plot the Laguerre tessellation
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figure
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patchpolygons(polys,cellids,myc);
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view([-37.5,30])
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axis equal
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axis off
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