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% Example_4_1.m
%
% This is Example 4.1 from the paper 'Geometric modelling of
% polycrystalline materials: Laguerre tessellations and periodic
% semi-discrete optimal transport' by D.P. Bourne, M. Pearce & S.M. Roper.
%
% We generate a 3D periodic Laguerre diagram with 10,000 grains of given
% volumes, where the grain volumes are drawn from a log-normal
% distribution, using the algorithm from Section 4 of the above paper.

clear

tic

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

n=10000; % number of grains

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% 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=2; % 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, which are drawn from a
% log-normal distribution

stdev=0.35; % standard deviation

% Define the log-normal parameter sigma, which is related to the standard
% deviation by stdev=sqrt(exp(Sigma^2)-1)
Sigma=sqrt(log(1+stdev^2)); % log-normal parameter sigma

% Define the log-normal parameter mu corresponding to mean=1
Mu=-0.5*Sigma^2;

% Draw the radii from the log normal distribution
radii=lognrnd(Mu,Sigma,[n,1]);
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% Calculate the corresponding grain volumes
% (note that we don't need the factor 4pi/3 as we'll be renormalising)
target_vols=radii.^3;

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

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% Perform the algorithm from Section 4 of the paper 'Geometric modelling
% of polycrystalline materials: Laguerre tessellations and periodic
% semi-discrete optimal transport' by D.P. Bourne, M. Pearce & S.M. Roper.

% Set the parameters of the algorithm
numLloyd=5; % number of regularisation (Lloyd) iterations
tol=1; % percentage error tolerance for the volumes of the grains

% Initialise the seed locations randomly
x0=L1*rand(n,1); % x-coordinates
y0=L2*rand(n,1); % y-coordinates
z0=L3*rand(n,1); % z-coordinates
Y=[x0,y0,z0]; % initial seed locations

% Initialise the weights
w=zeros(n,1);

% Iterative method
for m=1:numLloyd

    % 1. Regularisation step: move the seeds to the centroids of the grains
    [~,~,Y]=mexPD(bx,Y,w,periodic);
    % 2. Damped Newton step: find weights w so that grains have target vols
    [w,percent_error,actual_vols,~]=...
        SDOT_damped_Newton(zeros(n,1),Y,target_vols,bx,periodic,tol);

end

% Output the difference (percentage error) between the actual volumes of
% the grains and the target volumes
disp(strcat('Maximum percentage error=',num2str(percent_error),'%'));
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Maximum percentage error=0.06014%
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toc
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Elapsed time is 104.848800 seconds.
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% Plot the volume errors

percentage_errors=100*abs(actual_vols-target_vols)./target_vols;
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plotErrors(percentage_errors);
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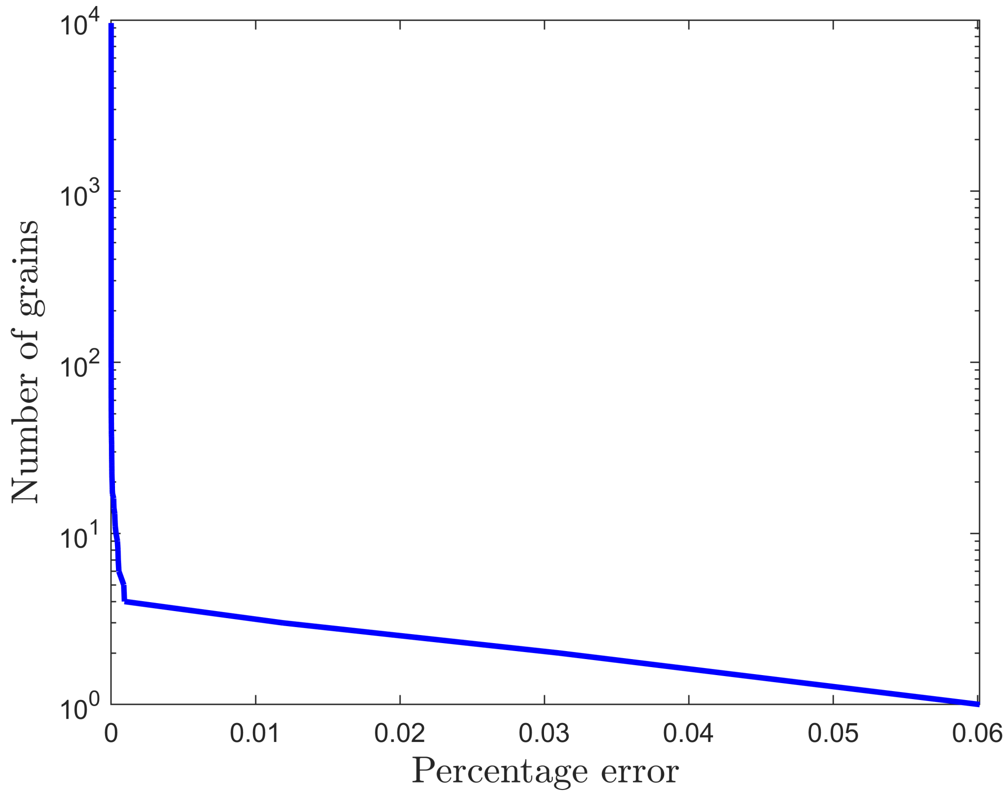


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% Plot the Laguerre tessellation

% Compute the vertices, faces, neighbours (vfn) of the Laguerre diagram
[~,~,~,vfn]=mexPDall(bx,Y,w,periodic);

% Compute which cells lie on the boundary of the box (no need to plot the
% interior cells since they are not visible)
[polys,cellids]=intersect_cells_on_boundary_periodic(bx,vfn);

% Colour the grains according to their volume, using a log scale
colormap=parula;
myc=generateGrainColours(log(actual_vols));

% Plot the Laguerre tessellation
figure
patchpolygons(polys,cellids,myc);
view([-37.5,30])
axis equal
axis off
```