true-particle-dynamics-model-of-Cahn-Hilliard-eq. 1, 1644, 1

```
In [1]:
       using VoronoiDelaunay
       using VoronoiCells
       using GeometryBasics
       using LinearAlgebra
       using Plots
       using ProgressMeter
       using JLD2
```

```
In [2]: import LinearAlgebra: norm
      norm(x::Point2D) = norm([x._x, x._y])
      # 距離がとても近い = ほぼ一致する, という判断を下す関数.
      function close(x,y)
         dist = norm(x - y)
         if dist < 1.5*eps()
             return true
         else
             return false
         end
      end
      # Point list の中の, どの point に該当するかを返す関数. 上の close関数を使う.
      function findpt(pts, pt)
         for i in 1:length(pts)
             if close(pts[i], pt)
                return i
             end
         end
         return 0 # false を返したいが、後で扱いにくいので、見つからない場合は 0 を返す.
      end
```

Out [2]: findpt (generic function with 1 method)

初期値等

```
In [3]: m = 0.005 # 粒子の大きさ.
      # Cahn-Hilliard eq. のパラメータ.
      p = -1.0
      q = -0.001
      r = 1.0
```

Out [3]: 1.0

(初期の) 点配置を作成する

[0.6751600742319119, 0.7806826862192365]

```
In [4]: # generator 情報は以下のようなものを想定する
        xmin, xmax = 0.0, 1.0
        width = xmax - xmin
        rect = Rectangle(Point2(xmin, xmin), Point2(xmax, xmax))
        # points = [Point2(width*rand()+xmin, width*rand()+xmin) for _ in 1:numpts]
        # ball の半径.この ball 内にはせいぜい1点しか入らないようにしたい.
        rb = 0.02
Out [4]: 0.02
In [5]: function make_pts(num)
            pmin = xmin + 0.15
            pwid = width - 0.3
            randp() = pwid * rand() + pmin
            pts = [ Point2( randp(), randp() ) ]
            for i in 2:num
               isadd = false
               while !(isadd)
                   candidate = Point2( randp(), randp() )
                   for j in 1:length(pts)
                       1 = norm(pts[j] - candidate)
                       if 1 < 2*rb
                           isadd = false
                           break
                       else
                           isadd = true
                       end
                   end
                   if isadd
                       push!(pts, candidate)
                   end
               end
          end
            return pts
        end
Out [5]: make_pts (generic function with 1 method)
In [6]:
        points = make_pts(60)
Out [6]: 60-element Vector{Point2{Float64}}:
        [0.6393563949703913, 0.652354442580869]
        [0.7918059513463728, 0.6812158503584586]
        \hbox{\tt [0.4926580774738232, 0.7945260289398132]}
        [0.7655352844695151, 0.7328820394325856]
```

```
[0.4225218020636574, 0.529979212857107]
[0.25674546325968894, 0.5133640149588149]
[0.653042818017378, 0.41243852358881194]
[0.47195505172150864, 0.6685803074103629]
[0.8137701676282519, 0.8373687882736839]
[0.7965785368136483, 0.1867135630022065]
[0.6839749479997027, 0.32006011670180895]
[0.2382711049584941, 0.6931227817386684]
[0.3910743970193288, 0.6655738894227181]
[0.6135597102203856, 0.15286464048193513]
[0.2558745887657953, 0.7438024595429749]
[0.49376239417341217, 0.7463573947398644]
[0.3849657404812351, 0.792363663803519]
[0.5618232499433176, 0.1953045086473449]
[0.3067689421517944, 0.7527887798182265]
[0.6861561944179245, 0.2281652359806733]
[0.1813748187362056, 0.5692652181353474]
[0.21911049024917337, 0.42306726558077346]
[0.3183205531930843, 0.2840126926914137]
[0.767310816401156, 0.45300698608500156]
```

VoronoiDelaunay, VoronoiCells pkg で points に対して様々な Voronoi 情報を計算する.

```
In [7]: # VoronoiDelauney を含め、幾何的ライブラリは、座標が 1+ε 以上 2 - 2ε 以下であるよう
      # 制限されていることが多い.
      # さらに, VD は余計な4隅の点を generator として勝手に加えてしまうので,
      # その影響を避けるため全体を小さくする変換関数、と逆変換を用意する.
      # 具体的には,全体を 4/3 = 1.333... から 5/3 = 1.666... の範囲に収まるように線形変搏
      # 幅は 5/3 - 4/3 = 1/3 になるので,元の幅を width とすると,縮小率は 1/(3 width) と
      rate_12sp = 1.0/(3*width) # これが縮小率.
      origin 12sp = 4.0/3 # 12sp の範囲の左端の値.
      function limit_to_12sp(x, xmin, xmax)
       return rate_12sp * (x - xmin) + origin_12sp
      end
      # 逆に戻す.
      function expand_from_12sp(x, xmin, xmax)
       return (x - origin 12sp)/rate 12sp + xmin
      end
      #座標 (x,y) を渡しての変換.
      limit_to_12sp(v::Point2, xmin, xmax) =
       Point2D( limit_to_12sp(v[1], xmin, xmax), limit_to_12sp(v[2], xmin, xmax) )
      expand from 12sp(v::Point2, xmin, xmax) =
       Point2D( expand_from_12sp(v[1], xmin, xmax), expand_from_12sp(v[2], xmin, xmax)
```

Out [7]: expand_from_12sp (generic function with 2 methods)

Points をもらって Voronoi の様々な情報を計算する 1stop関数.

```
In [8]: # それがこれ.
```

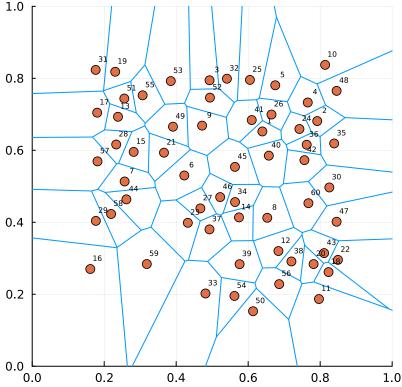
```
function make_cx_l(pts)
   num = length(pts)
   pts 12 = [ limit to 12sp( pts[n], xmin, xmax ) for n in 1:num ]
   tess = DelaunayTessellation()
   push!( tess, copy(pts_12) )
   # DelaunayTesselation は渡した点の順番を変えてしまうのでコピーを渡す.
   veds = voronoiedges(tess) # Voronoi Edges
   deds = delaunayedges(tess) # Delaunay Edges
   # 一応, お絵かきのために.
   x, y = getplotxy(veds)
   ox = [ expand_from_12sp( x[i], xmin, xmax) for i in 1:length(x) ]
   oy = [ expand_from_12sp( y[i], xmin, xmax) for i in 1:length(y) ]
   # この ox, oy を返しておく.
   # お絵かきは次のような感じで.
   # plot(ox, oy, xlims = (0,1.0), ylims = (0,1.0), aspect_ratio = 1.0)
   # scatter!(pts, markersize = 4, label = "generators", aspectratio = 1.0)
   # annotate!([(pts[n][1] + 0.02, pts[n][2] + 0.03, Plots.text(n)) for n in 1:n
   edgepts = [ (geta(edge), getb(edge)) for edge in deds ]
   # delaunay edge の端点を全て列挙する.
   omatc = zeros(Bool, num, num)
   for n in 1:length(edgepts) # 連結行列を作る
       pa, pb = edgepts[n][1], edgepts[n][2]
       i, j = findpt(pts_12, pa), findpt(pts_12, pb)
       omatc[i,j] = omatc[j,i] = true
   end
   omatl = zeros(num, num) # 本来の座標系での真の格子点間距離
   for i in 1:num
       for j in (i+1):num
          if omatc[i,j] # ただし連結行列で繋がっている場合のみ.
              omatl[i,j] = omatl[j,i] = norm( pts[i] - pts[j] )
          end
       end
   end
   # Voronoi 境界線の長さ、本来の長さに直している.
   # VoronoiEdges から取り出した edge は、その edge を通じて Voronoi領域が接する格
   # generator として持っている.
   # それらは、getgena(), getgenb() で取り出せる.
   # Voronoi cell の境界面の真の長さ r_{ij}
   omatr = zeros(num, num)
   for edge in veds
     i,j = findpt( pts_12, getgena(edge) ), findpt( pts_12, getgenb(edge) )
     if (i*j > 0) && omatc[i,j]
       # 上で見つけた i or j が Voronoi のテクニカルな仮想点相当の場合(findpt が 0
       # あともちろん、連結行列で繋がっているときのみ.
       omatr[i,j] = omatr[j,i] = norm( geta(edge) - getb(edge) ) / rate_12sp
       # tess は large2small で小さくなっているので、戻す
```

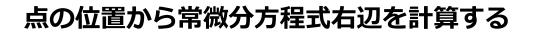
```
end
            end
            # VoronoiCells の方の機能でもう一度分割することになるが,各 Voronoi Cell の面積
            # しかも、縮小していない状態なので、値を拡大縮小で戻したりする必要がない.
            ov = voronoiarea(voronoicells(pts, rect))
            return (ox, oy, omatc, omatl, omatr, ov)
        end
Out [8]: make_cx_l (generic function with 1 method)
 In [9]:
        (ox, oy, omatc, omatl, omatr, ov) = make_cx_l(points);
In [10]:
        omatc
Out [10]: 60×60 Matrix{Bool}:
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In [11]:
           omatl
Out [11]: 60×60 Matrix{Float64}:
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 In [12]:
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Out [12]: 60×60 Matrix{Float64}:
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 In [13]:
           ον
Out [13]: 60-element Vector{Float64}:
           0.004933657961751669
           0.005409549629229002
           0.016520941247671277
           0.007340133224112033
           0.0144478353527281
           0.013605819146154836
           0.00809569021726865
           0.011973526188179442
           0.011543677616035516
           0.052369355493841016
           0.055190573728010714
           0.008609759709967026
           0.005801482050128377
           0.009898085314043546
           0.03492134095424768
           0.004649093246856865
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0.008503935546570949
          0.010787725049078978
          0.030054945410406098
          0.008879375879362909
          0.04013229416208567
          0.011729981949758696
 In [14]:
          m ./ ov
Out [14]: 60-element Vector{Float64}:
          1.0134468256135
          0.9242913629970019
          0.3026461946110231
          0.6811865462571179
          0.34607260381437555
          0.3674898178705439
          0.6176125649341998
          0.41758792868688277
          0.4331375291574685
          0.09547568330467679
          0.09059518070315628
          0.5807363002490983
          0.861848740855685
          0.505148202037209
          0.1431789233566594
          1.0754785362458312
          0.6765088376841946
          0.1778318356846806
          0.5631519965159785
          0.5879630639976047
          0.4634897512916205
          0.16636197243828035
          0.5631026400876665
          0.12458794356001876
          0.4262581154357921
 In [15]:
          plot(ox, oy, xlims = (0,1.0), ylims = (0,1.0), aspect_ratio = 1.0, legend = false
          scatter!(points, markersize = 5, label = "generators", aspectratio = 1.0)
          annotate!([(points[n][1] + 0.02, points[n][2] + 0.03, Plots.text(n, 5)) for n in
Out [15]:
```

 $\begin{array}{c} \textbf{0.007390886447420045} \\ \textbf{0.028116450469901588} \\ \textbf{0.008878597662679392} \end{array}$





```
In [16]: function rhs(pts, mat_c, mat_l, mat_r, vol )
            num = length(pts)
            u = m ./ vol # 各 cell での密度.
            # phi = delta G/ delta u
            tilu = 2.0 .* u .- 1.0
            phi = similar(u)
            for i in 1:num
                if abs(tilu[i]^2) < (-p/r)
                    phi[i] = p * tilu[i] + r * (tilu[i]^3)
                    phi[i] = u[i] > 0.5 ? 100.0 : -100.0 # 本来はここは sign * ∞.
                end
            end
            mat_B = zeros(num, num)
            for i in 1:num
                for j in i+1:num
                    if mat_c[i,j]
                        mat_B[i,j] = mat_B[j,i] = mat_r[i,j]/mat_l[i,j]
                    end
                end
            end
            lapl_u = similar(u)
            one_v = ones(num)
            for i in 1:num
                lapl_u[i] = dot( mat_B[i, :], u - u[i] .* one_v ) / vol[i]
            end
            lapl_u = (2*q) .* lapl_u
            phi = phi + lapl_u
            v = [0.0, 0.0] for i in 1:num ]
            for i in 1:num
                for j in 1:num
                    if mat_c[i,j]
                        v[i] += ( phi[j] * mat_r[i,j] / mat_l[i,j] ).* (pts[j] - pts[i])
                    end
                end
            end
            v = (-1/(2*m)) .* v
            return v
        end
```

```
Out [16]: rhs (generic function with 1 method)

In [17]: rhs( points, omatc, omatl, omatr, ov)
```

```
Out [17]: 60-element Vector{Vector{Float64}}:
           [-245.48884372939602, -14.707803184370338]
          [569.616890781495, 443.55822089345713]
          [-13.939748696889016, -3.2672621226395866]
          [117.28017730458488, 376.9430792851558]
          [5.213367755854972, -3.5638295783363567]
          [-2.433167932586879, 4.077182359403438]
          [3.083229251105293, 1.7965206203703608]
          [-2.5296973643971854, -3.7200128717937666]
          [1.854980272848292, -0.150067628533173]
          [43.53485389339326, 42.44549924874684]
          [72.57368201910704, -342.045447287739]
          [-915.7098744345566, 732.4539333621323]
          [-254.93733122135995, -744.5723146410245]
          [-2.7000937988941307, -1.7047126471819458]
          [12.893239146297844, -16.50586796108903]
[4.103542626166358, -3.7972809354477928]
          [1.0965045544112522, -5.711840379282376]
          [4.704033762602654, -7.39879982178128]
          [-0.34147910176961865, 1.8001302409432047]
          [884.0580897847929, 152.4645639132362]
          [-447.3844982815, -727.9160193612598]
          [-0.2528152006543918, 3.190068209999934]
          [4.952071977652846, 4.8247037775965795]
          [-1.5637397217559648, 1.4306023294306347]
          [-5.4614134784516795, 2.683569836257812]
         時間発展は Runge-Kutta 法で.
In [18]:
         function rhs(points)
               (ox, oy, omatc, omatl, omatr, ov) = make_cx_l(points)
               return rhs( points, omatc, omatl, omatr, ov)
          end
Out [18]: rhs (generic function with 2 methods)
In [19]: function RK(u)
               r1 = rhs(u)
               r2 = rhs(u + \Delta t/2 * r1)
               r3 = rhs(u + \Delta t/2 * r2)
              r4 = rhs(u + \Delta t * r3)
               return u + \Deltat * (r1 + 2*r2 + 2*r3 + r4)/6
          end
Out [19]: RK (generic function with 1 method)
In [20]:
          \Delta t = 0.00000005
          u0 = copy(points)
          u = u0 # 最初の値はもちろん初期値
          u_sq = [ u ] # 初期値を配列に入れておいて...
          @showprogress for n in 1:30000
               u = RK(u) # Runge-Kutta 法で新しい値をいきなり求める.
               push!(u_sq, u) # その値を配列に追加していく.
          end
          [32mProgress: 100%|
                                                                   | Time: 0:04:19[39mmmm9m
```

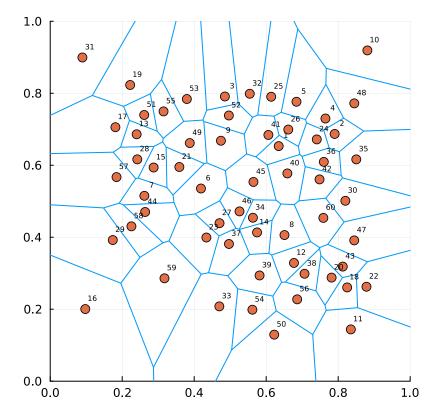
In [21]:

u_sq[end]

```
Out [21]: 60-element Vector{Point2{Float64}}:
           [0.6347572647300732, 0.653219436909223]
           [0.7901954558905152, 0.686989565794952]
           [0.48524425615188044, 0.7911061203819574]
           [0.7645945609139676, 0.729848598591848]
           [0.6841042455169657, 0.7764077314674231]
           [0.41876108688025954, 0.5353911449488652]
           [0.2615559094112178, 0.5151126655425453]
           [0.6508222139762806, 0.4060643954588918]
           [0.4742848121484637, 0.6681327583484503]
           [0.881088336409271, 0.9190977028053389]
            [0.8351535146907376, 0.14393000909299472]
           [0.6771741476898018, 0.32861447161016094]
           [0.24012112719206583, 0.6860892267445078]
           [0.38772822611053737, 0.6616900643806227]
           [0.6223363168924433, 0.12931299116738135]
           [0.2610918873033611, 0.7397169938474597]
           [0.4963388220726547, 0.7382581075984584]
           [0.37960268673387904, 0.7840626385546914]
           [0.5616709759615586, 0.19861870496310136]
           \hbox{\tt [0.3148326106126286, 0.7496615773123936]}
           [0.6861085274144135, 0.227467242632074]
           [0.18420237332284228, 0.5671386804358902]
           [0.22562431293020593, 0.43033320836991806]
           [0.3174246247374079, 0.2859242018442965]
           [0.7587945114555679, 0.45377345039499334]
```

In [23]: (ox, oy, omatc, omatl, omatr, ov) = make_cx_l(u_sq[end]) plot(ox, oy, xlims = (0,1.0), ylims = (0,1.0), aspect_ratio = 1.0, legend = false scatter!(u_sq[end], markersize = 5, label = "generators", aspectratio = 1.0) annotate!([(u_sq[end][n][1] + 0.02, u_sq[end][n][2] + 0.03, Plots.text(n, 5)) for

Out [23]:

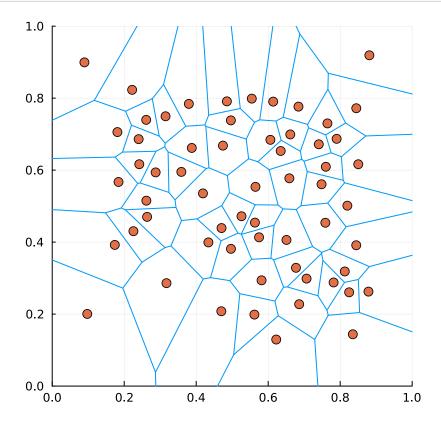


```
In [24]: function view_v_noanon(pts)
   (ox, oy, omatc, omatl, omatr, ov) = make_cx_l(pts)
   plot(ox, oy, xlims = (0,1.0), ylims = (0,1.0), aspect_ratio = 1.0, legend = fal
   scatter!(pts, markersize = 5, label = "generators", aspectratio = 1.0)
end
```

Out [24]: view_v_noanon (generic function with 1 method)

```
In [25]: view_v_noanon( u_sq[end] )
```

Out [25]:



```
In [26]: using Printf # すぐ下の @sprintf を使いたいので.

function figure(dir, n_skip, num)
    true_num = num * n_skip
    s = @sprintf("%8.7f", true_num * Δt)

    (ox, oy, omatc, omatl, omatr, ov) = make_cx_l(u_sq[true_num+1])
    plot(ox, oy, xlims = (0,1.0), ylims = (0,1.0), aspect_ratio = 1.0, legend = f
    scatter!(u_sq[true_num+1], markersize = 5, label = "generators", aspectratio
    # 時間をタイトルに表示

    savefig( dir * "/" * @sprintf("%06d", num) * ".png" )
    # 6桁の数字.png というファイル名で保存
end
```

```
In [27]: dir = "true-pd-60pts"
  run(`cmd /k mkdir $dir`)
```

c:\home\julia-programs\v1.9>

Out [26]: figure (generic function with 1 method)

Out [27]: Process(`[4mcmd[24m [4m/k[24m [4mmkdir[24m [4mtrue-pd-60pts[24m`, ProcessExited(0))

Hey there! If you have any feedback for this tool - issues, ideas for improvement, or you want to just tell me about your use case for this, I'd love to know. <u>E-mail me</u> or <u>tweet at me</u>.