Interior cells

Cell geometry

Piecewise constant variables

Auxiliary functions

$$\begin{aligned} &\text{Rules} \ = \Big\{ \frac{h^c_{\ i} \ u_i}{D_i} \ -> Pe_i, \ \frac{h^c_{\ i+1} \ u_{i+1}}{D_{i+1}} \ -> Pe_{i+1}, \ \frac{h^c_{\ i-1} \ u_{i-1}}{D_{i-1}} \ -> Pe_{i-1}, \ \frac{h^c_{\ 1} \ u_1}{D_1} \ \rightarrow Pe_1, \ \frac{h^c_{\ N} \ u_N}{D_N} \ \rightarrow Pe_N \Big\}; \\ &\text{Rules2} \ = \Big\{ Pe_{1+j} \ \rightarrow \ \frac{h^c_{\ j+1} \ u_{j+1}}{D_{j+1}}, \ Pe_j \ \rightarrow \ \frac{h^c_{\ j} \ u_j}{D_j}, \ Pe_{j-1} \ \rightarrow \ \frac{h^c_{\ j-1} \ u_{j-1}}{D_{j-1}}, \ Pe_1 \ \rightarrow \ \frac{h^c_{\ 1} \ u_1}{D_1}, \ Pe_2 \ \rightarrow \ \frac{h^c_{\ 2} \ u_2}{D_2}, \ Pe_N \ \rightarrow \ \frac{h^c_{\ N} \ u_N}{D_N}, \\ &Pe_{N-1} \ \rightarrow \ \frac{h^c_{N-1} \ u_{N-1}}{D_{N-1}} \Big\}; \end{aligned}$$

Λ in equation (3), Llorente 2020 AMC

$$\begin{aligned} & \text{pintgr}_{j+1/2}[z_{-}, i_{-}] = \text{Assuming} \Big[\text{Between} \Big[z, X_{i+\frac{1}{2}} \Big], \text{ FullSimplify} \Big[\int_{x_{i}+\frac{1}{2}h^{c}_{i}}^{z} \frac{u[t, i]}{Df[t, i]} \, dt \Big] \Big] \\ & \text{pintgr}_{j-1/2}[z_{-}, i_{-}] = \text{Assuming} \Big[\text{Between} \Big[z, X_{i-\frac{1}{2}} \Big], \text{ FullSimplify} \Big[\int_{x_{i}-\frac{1}{2}h^{c}_{i}}^{z} \frac{u[t, i]}{Df[t, i]} \, dt \Big] \Big] \\ & \\ & \left[-\frac{u_{i} \left(-2z + h^{c}_{i} + 2x_{i} \right)}{2D_{i}} \quad 2z < h^{c}_{i} + 2x_{i} \\ -\frac{u_{1+i} \left(-2z + h^{c}_{i} + 2x_{i} \right)}{2D_{1+i}} \quad 2z > h^{c}_{i} + 2x_{i} \\ 0 & \text{True} \\ \end{aligned} \right]$$

```
 \text{Out[*]=} \left\{ \begin{array}{l} \frac{u_{-1+i} \left(2 \, z + h^{c}_{i} - 2 \, x_{i}\right)}{2 \, D_{-1+i}} & 2 \, z + h^{c}_{i} < 2 \, x_{i} \\ \frac{u_{i} \left(2 \, z + h^{c}_{i} - 2 \, x_{i}\right)}{2 \, D_{i}} & 2 \, z + h^{c}_{i} > 2 \, x_{i} \\ 0 & \text{True} \end{array} \right.
```

S in equation (3), Llorente 2020 AMC

$$S^{\text{intgr}}_{j-1/2}[z_{-}, i_{-}] = \text{Assuming}\left[\text{Between}\left[z, X_{i-\frac{1}{2}}\right], \text{FullSimplify}\left[\int_{x_{i}-\frac{1}{2}}^{z} S[t, i] dt\right]\right]$$

$$\text{Out[o]=} \left\{ \begin{array}{l} \frac{1}{2} \, S_{i} \, \left(2 \, z - h^{c}{}_{i} - 2 \, x_{i} \right) \, \phi_{i} & 2 \, z < h^{c}{}_{i} + 2 \, x_{i} \\ \frac{1}{2} \, S_{1+i} \, \left(2 \, z - h^{c}{}_{i} - 2 \, x_{i} \right) \, \phi_{1+i} & 2 \, z > h^{c}{}_{i} + 2 \, x_{i} \\ 0 & \text{True} \end{array} \right.$$

Out[*]=
$$\begin{cases} \frac{1}{2} S_{-1+i} & (2 z + h^{c}_{i} - 2 x_{i}) \phi_{-1+i} & 2 z + h^{c}_{i} < 2 x_{i} \\ \frac{1}{2} S_{i} & (2 z + h^{c}_{i} - 2 x_{i}) \phi_{i} & 2 z + h^{c}_{i} > 2 x_{i} \\ 0 & \text{True} \end{cases}$$

 $<\lambda$, 1> in equation (6), Llorente 2020 AMC

$$Pe_{j+1/2}[i_{-}] = FullSimplify \left[\int_{x_{i}}^{x_{i}+\frac{1}{2}h^{c}_{i}+\frac{1}{2}h^{c}_{i+1}} \frac{u[z, i]}{Df[z, i]} dz \right]$$

$$Pe_{j-1/2}[i_{-}] = FullSimplify \left[\int_{x_{i}-\frac{1}{2}h^{c}_{i}-\frac{1}{2}h^{c}_{i-1}}^{x_{i}} \frac{u[z, i]}{Df[z, i]} dz \right]$$

Out[
$$\circ$$
]= $\frac{1}{2} \left(\frac{h^{c}_{-1+i} u_{-1+i}}{D_{-1+i}} + \frac{h^{c}_{i} u_{i}}{D_{i}} \right)$

 $<\lambda, e^{-\Lambda}>$ in equation (6), Llorente 2020 AMC

$$Intgr^{pe}_{j+1/2}[i_{-}] = FullSimplify \left[\int_{x_{i}}^{x_{i}+\frac{1}{2}h^{c}_{i}+\frac{1}{2}h^{c}_{i+1}} \frac{u[z, i]}{Df[z, i]} Exp \left[-p^{intgr}_{j+1/2}[z, i] \right] dz \right]$$

$$Intgr^{pe}_{j-1/2}[i_{-}] = FullSimplify \left[\int_{x_{i}-\frac{1}{2}h^{c}_{i-1}}^{x_{i}} \frac{u[z, i]}{Df[z, i]} Exp \left[-p^{intgr}_{j-1/2}[z, i] \right] dz \right]$$

$$Out[s] = \begin{bmatrix} \frac{h^{c}_{i}u_{i}}{2D_{i}} - e^{-\frac{h^{c}_{1+i}u_{1+i}}{2D_{1+i}}} \\ e^{\frac{h^{c}_{-1+i}u_{-1+i}}{2D_{-1+i}} - e^{-\frac{h^{c}_{i}u_{i}}{2D_{i}}} \end{bmatrix}$$

 $<\Gamma^{-1}$, $e^{-\Lambda}>$ in equation (6), Llorente 2020 AMC

$$Intgr^{D}_{j+1/2}[i_{-}] = FullSimplify \left[\int_{x_{i}}^{x_{i} + \frac{1}{2} h^{C}_{i} + \frac{1}{2} h^{C}_{i+1}} \frac{1}{Df[z, i]} Exp \left[-p^{intgr}_{j+1/2}[z, i] \right] dz \right]$$

$$Intgr^{D}_{j-1/2}[i_{-}] = FullSimplify \left[\int_{x_{i} - \frac{1}{2} h^{C}_{i-1}}^{x_{i}} \frac{1}{Df[z, i]} Exp \left[-p^{intgr}_{j-1/2}[z, i] \right] dz \right]$$

$$Out[s] = \frac{-1 + e^{\frac{h^{C}_{i} u_{i}}{2D_{i}}}}{u_{i} \phi_{i}} + \frac{1 - e^{-\frac{h^{C}_{1+i} u_{1+i}}{2D_{1+i}}}}{u_{1+i} \phi_{1+i}}$$

$$\frac{-1 + e^{\frac{h^{c}_{-1+i} u_{-1+i}}{2 D_{-1+i}}}}{u_{-1+i} \phi_{-1+i}} + \frac{1 - e^{-\frac{h^{c}_{i} u_{i}}{2 D_{i}}}}{u_{i} \phi_{i}}$$

 $< S\Gamma^{-1}, e^{-\Lambda} >$ in equation (6), Llorente 2020 AMC

Out[•]=

Intgr^S_{j+1/2} [i] = FullSimplify
$$\left[\int_{x_i}^{x_i + \frac{1}{2}h^c_{i} + \frac{1}{2}h^c_{i+1}} \frac{S^{intgr}_{j+1/2}[z, i]}{Df[z, i]} Exp\left[-P^{intgr}_{j+1/2}[z, i] \right] dz \right]$$

$$S^{intgr}_{j-1/2}[z, i] = S^{intgr}_{j-1/2}[z, i] = S^{in$$

Intgr^S_{j-1/2} [i_] = FullSimplify
$$\left[\int_{x_{i}-\frac{1}{2}h^{c}_{i}-\frac{1}{2}h^{c}_{i-1}}^{x_{i}} \frac{S^{intgr}_{j-1/2}[z, i]}{Df[z, i]} \exp \left[-P^{intgr}_{j-1/2}[z, i] \right] dz \right]$$

$$\textit{Out[@]=} \quad \frac{\left(-1 + \mathbb{Q}^{\frac{h^{c}_{i} \, u_{i}}{2 \, D_{i}}} \right) \, D_{i} \, S_{i}}{u_{i}^{2}} \, + \, \frac{1}{2} \left(-\frac{\frac{h^{c}_{i} \, u_{i}}{2 \, D_{i}} \, h^{c}_{i} \, S_{i}}{u_{i}} \, + \, \frac{S_{1+i} \left(2 \, D_{1+i} \, - \, \mathbb{Q}^{-\frac{h^{c}_{1+i} \, u_{1+i}}{2 \, D_{1+i}}} \, (2 \, D_{1+i} \, + \, h^{c}_{1+i} \, u_{1+i}) \right)}{u_{1+i}^{2}} \right)$$

$$\frac{\mathrm{e}^{-\frac{h^{c}_{\mathbf{i}}\,u_{\mathbf{i}}}{2\,D_{\mathbf{i}}}}\left(2\,\left(-1+\mathrm{e}^{\frac{h^{c}_{\mathbf{i}}\,u_{\mathbf{i}}}{2\,D_{\mathbf{i}}}}\right)\,D_{\mathbf{i}}\,S_{\mathbf{i}}\,u_{-1+\mathbf{i}}^{2}+u_{\mathbf{i}}\,\left(-h^{c}_{\mathbf{i}}\,S_{\mathbf{i}}\,u_{-1+\mathbf{i}}^{2}+\mathrm{e}^{\frac{h^{c}_{\mathbf{i}}\,u_{\mathbf{i}}}{2\,D_{\mathbf{i}}}}\,S_{-1+\mathbf{i}}\,\left(-2\,D_{-1+\mathbf{i}}+\mathrm{e}^{\frac{h^{c}_{-1+\mathbf{i}}\,u_{-1+\mathbf{i}}}{2\,D_{-1+\mathbf{i}}}}\,(2\,D_{-1+\mathbf{i}}-h^{c}_{-1+\mathbf{i}}\,u_{-1+\mathbf{i}})\,\right)\,u_{\mathbf{i}}\right)\right)}{2\,u_{-1+\mathbf{i}}^{2}\,u_{-1+\mathbf{i}}^{2}\,u_{-1+\mathbf{i}}^{2}}$$

ln[=]:= $B[z_{-}] = z / (Exp[z] - 1);$

Out[•]=

Fluxes

Homogeneous flux

Equation (6), Llorente 2020 AMC

$$F^{H}_{i+\frac{1}{2}} = \frac{\langle \lambda, e^{-\Lambda} \rangle / \langle \lambda, 1 \rangle}{\langle \Gamma^{-1}, e^{-\Lambda} \rangle} [B(-\langle \lambda, 1 \rangle) C_{i} - B(\langle \lambda, 1 \rangle) C_{i+1}]$$

$$F^{I}_{i+\frac{1}{2}} = -\frac{\langle S\Gamma^{-1}, e^{-\Lambda} \rangle}{\langle \Gamma^{-1}, e^{-\Lambda} \rangle}$$

Inhomogeneous flux

Total flux

```
\Delta F_{j}[i_{-}] = Collect[F^{H}_{j-1/2}[i] - F^{H}_{j+1/2}[i] + F^{I}_{j-1/2}[i] - F^{I}_{j+1/2}[i], \{C_{i-1}, C_{i}, C_{i+1}, S_{i-1}, S_{i}, S_{i+1}\}, Simplify];
```

Boundary conditions

x @ 0

```
Y[X] =
 In[•]:=
                        y[x] /. First@DSolve[{-D_1 \phi_1 * y''[x] + u_1 \phi_1 * y'[x] = S_1 \phi_1, \alpha_0 * y[0] + \beta_0 * y'[0] = \gamma_0, y[h^c_1/2] = C_1}, y[x], x];
                   F_{\underline{1}} = Collect[-D_1 \phi_1 * Y'[0] + u_1 \phi_1 * Y[0], \{C_1, S_1, r_0\}, Simplify] /. Rules;
                   F_{\frac{1}{2}} == A_{m1}[1] * C_1 + B_{m1}[1] * S_1 + b[1] /. Rules2 // Simplify
 In[•]:=
                   True
Out[•]=
             F_{\frac{1}{2}}^{H} = Coefficient \left[F_{\frac{1}{2}}, \{C_1\}\right] * C_1
                  F^{I}_{\frac{1}{2}} = FullSimplify \left[ Coefficient \left[ F_{\frac{1}{2}}, \{S_{1}\} \right] \right] * S_{1}
                   \Delta F_{1}^{H} = F_{\frac{1}{2}}^{H} - F_{j+1/2}^{H}[1] /. Rules;
                   \Delta F_{1}^{I} = F_{\frac{1}{2}}^{I} - F_{j+1/2}^{I}[1] /. Rules;
Out[\bullet] = \left\{ \begin{array}{c|c} C_1 u_1 & (D_1 \alpha_0 + u_1 \beta_0) & \phi_1 \\ \hline - \left( -1 + e^{\frac{Pe_1}{2}} \right) D_1 \alpha_0 + u_1 \beta_0 \end{array} \right\}
 Out[\bullet] = \left\{ \begin{array}{l} S_1 \left( 2 \left( -1 + e^{\frac{Pe_1}{2}} \right) D_1 - h^c_1 u_1 \right) \left( D_1 \alpha_0 + u_1 \beta_0 \right) \phi_1 \\ 2 u_1 \left( -\left( -1 + e^{\frac{Pe_1}{2}} \right) D_1 \alpha_0 + u_1 \beta_0 \right) \end{array} \right\}
```

```
8 | fvcf.nb
X @ L
```

```
Z[x_{-}] = z[x] / . \text{ First @ DSolve} \left[ \left\{ -D_{N} \phi_{N} * z''[x] + u_{N} \phi_{N} * z'[x] = S_{N} \phi_{N}, \ \alpha_{L} * z[L] + \beta_{L} * z'[L] = \gamma_{L}, \ z[L - h^{c}_{N}/2] = C_{N} \right\},
z[x], x];
F_{N+\frac{1}{2}} = \text{Collect}[-D_{N} \phi_{N} * Z'[L] + u_{N} \phi_{N} * Z[L], \{C_{N}, S_{N}, r_{L}\}, \text{ Simplify}] / . \text{ Rules};
```

In[
$$\phi$$
]:=
$$F_{N+\frac{1}{2}}^{H} = \text{Coefficient}\left[F_{N+\frac{1}{2}}, \{C_{N}\}\right] * C_{N};$$

$$F_{N+\frac{1}{2}}^{I} = \text{FullSimplify}\left[\text{Coefficient}\left[F_{N+\frac{1}{2}}, \{S_{N}\}\right]\right] * S_{N};$$

$$\Delta F_{N}^{H} = F_{j+1/2}^{H}[N-1] - F_{N+\frac{1}{2}}^{H} / . \text{ Rules};$$

$$\Delta F_{N}^{I} = F_{j+1/2}^{I}[N-1] - F_{N+\frac{1}{2}}^{I} / . \text{ Rules};$$

Matrix form

$$\Delta F = A*C + B*S + b$$

Boundary terms

 $[b_1, 0, ..., 0, b_N]$

$$b[1] = \frac{D_1 u_1 \gamma_0 \phi_1}{-D_1 \alpha_0 e^{-\frac{Pe_1}{2}} + D_1 \alpha_0 - u_1 \beta_0 e^{-\frac{Pe_1}{2}}};$$

$$b[N] = \frac{e^{-\frac{Pe_N}{2}} D_N u_N \gamma_L \phi_N}{-D_N \alpha_L e^{-\frac{Pe_N}{2}} + D_N \alpha_L + u_N \beta_L};$$

$$b[1] - \text{Coefficient}[F_{\frac{1}{2}}, \gamma_0] * \gamma_0 // \text{Simplify}$$

$$b[N] - \left(-\text{Coefficient}[F_{N+\frac{1}{2}}, \gamma_L] * \gamma_L\right) // \text{Simplify}$$

$$Out[-] = \emptyset$$

Homogeneous terms

$$A \times C$$
, $A = [\ldots, A_{lower}, A_{ml} + A_{mu}, A_{upper}, \ldots]$

```
 \begin{aligned} &\text{Afun}[i_{-}] = \frac{u_{i} \phi_{i} \, u_{i+1} \, \phi_{i+1}}{\left(-e^{-\frac{Pe_{i}+Pe_{i+1}}{2}} + e^{-\frac{Pe_{i}}{2}}\right) \, u_{i} \, \phi_{i} + \left(1 - e^{-\frac{Pe_{i}}{2}}\right) \, u_{i+1} \, \phi_{i+1}}; \\ &\text{A}_{lower}[j_{-}] = \text{Afun}[j - 1]; \\ &\text{A}_{ml}[j_{-}] = -e^{-\frac{Pe_{-1+j}+Pe_{j}}{2}} \, \text{Afun}[j - 1]; \\ &\text{A}_{mu}[j_{-}] = -\text{Afun}[j]; \\ &\text{A}_{upper}[j_{-}] = e^{-\frac{Pe_{1}+Pe_{1+j}}{2}} \, \text{Afun}[j]; \end{aligned} 
 &\text{A}_{ml}[1] = \frac{u_{1} \, \phi_{1} \, (D_{1} \, \alpha_{0} + u_{1} \, \beta_{0}) \, e^{-\frac{Pe_{1}}{2}}}{D_{1} \, \alpha_{0} + u_{1} \, \beta_{0} \, e^{-\frac{Pe_{1}}{2}}}; \\ &\text{A}_{mu}[N] = \frac{u_{N} \, \phi_{N} \, (D_{N} \, \alpha_{L} + u_{N} \, \beta_{L})}{D_{N} \, \alpha_{L} \, e^{-\frac{Pe_{N}}{2}} - D_{N} \, \alpha_{L} - u_{N} \, \beta_{L}}; \end{aligned}
```

Interior cells

Out[*]= **0**

Out[*]= 0

Boundary cells

Boundary conditions only go into $A_{m1} [1]$ and $A_{mu} [N]$

```
\left(\mathsf{Coefficient}\left[\Delta\mathsf{F}^\mathsf{H}_{1}\texttt{[[1]]},\mathsf{C}_{1}\right]\ -\ \left(\mathsf{A}_{m1}\texttt{[1]}+\mathsf{A}_{mu}\texttt{[1]}\right)\right)\ /\ .\ \mathsf{Rules2}\ //\ \mathsf{Simplify}
In[•]:=
              (Coefficient \left[F^{H}_{\frac{1}{2}}[[1]], C_{1}\right] - A_{ml}[1]) /. Rules2 // Simplify
              (Coefficient \left[-F^{H}_{j+1/2}[1], C_{1}\right] - A_{mu}[1]) /. Rules2 // Simplify
              (Coefficient[\Delta F^{H}_{N}[[1]], C_{N}] - (A_{ml}[N] + A_{mu}[N])) / . Rules2 // Simplify
              (Coefficient [F^H_{j+1/2}[N-1], C_N] - A_{ml}[N]) /. Rules2 // Simplify
              (Coefficient \left[-F_{N+\frac{1}{2}}^{H}[[1]], C_{N}\right] - A_{mu}[N]) /. Rules2 // Simplify
             0
Out[•]=
             0
Out[•]=
             0
Out[•]=
             0
Out[•]=
             0
Out[•]=
             0
Out[•]=
```

Inhomogeneous terms

$$B \times S$$
, $B = [\ldots, B_{lower}, B_{ml} + B_{mu}, B_{upper}, \ldots]$

$$Bfun_{1}[i_{-}] = h^{c}_{i} \frac{e^{-\frac{Pe_{i}}{2}} + \frac{Pe_{i}}{2} - 1}{u_{i} Pe_{i} \left(\frac{1-e^{-\frac{Pe_{i}}{2}}}{u_{i} \phi_{i}} + \frac{e^{-\frac{Pe_{i}}{2}} - \frac{Pe_{i} + Pe_{1 + i}}{2}}{u_{1 + i} \phi_{1 + i}}\right)};$$

$$Bfun_{u}[i_{-}] = h^{c}_{i+1} \frac{e^{-\frac{Pe_{i}}{2}} - e^{-\frac{Pe_{i} + Pe_{1 + i}}{2}} - \frac{Pe_{1 + i}}{2} e^{-\frac{Pe_{1} + Pe_{1 + i}}{2}}}{u_{1 + i} Pe_{1 + i} \left(\frac{1-e^{-\frac{Pe_{i}}{2}}}{u_{i} \phi_{i}} + \frac{e^{-\frac{Pe_{i}}{2}} - \frac{Pe_{i} + Pe_{1 + i}}{2}}{u_{1 + i} \phi_{1 + i}}\right)};$$

$$Blower[j_{-}] = Bfun_{1}[j-1];$$

$$Bm_{1}[j_{-}] = -Bfun_{1}[j];$$

$$Bm_{1}[j_{-}] = -Bfun_{1}[j];$$

$$Bupper[j_{-}] = Bfun_{1}[j];$$

$$Bupper[j_{-}] = Bfun_{1}[j];$$

$$Bupper[j_{-}] = Bfun_{1}[j];$$

$$Bupper[j_{-}] = Bfun_{1}[j];$$

$$Bupper[j_{-}] = \frac{h^{c}_{1} \phi_{1} (D_{1} \alpha_{0} + u_{1} \beta_{0}) \left(1 - e^{-\frac{Pe_{1}}{2}} - \frac{Pe_{1}}{2} e^{-\frac{Pe_{1}}{2}}\right)}{Pe_{1} \left(D_{1} \alpha_{0} e^{-\frac{Pe_{1}}{2}} - D_{1} \alpha_{0} + u_{1} \beta_{0} e^{-\frac{Pe_{1}}{2}}\right)};$$

$$Buu[N] = \frac{h^{c}_{N} \phi_{N} (D_{N} \alpha_{L} + u_{N} \beta_{L}) \left(1 - e^{-\frac{Pe_{N}}{2}} - \frac{Pe_{N}}{2}\right)}{Pe_{N} \left(-D_{N} \alpha_{L} e^{-\frac{Pe_{N}}{2}} + D_{N} \alpha_{L} + u_{N} \beta_{L}\right)};$$

```
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                  \left( \mathsf{Coefficient} \left[ \Delta \mathsf{F}^{\mathsf{I}}_{\mathsf{j}} \left[ \mathsf{j} \right], \mathsf{S}_{\mathsf{j-1}} \right] - \mathsf{B}_{\mathsf{lower}} \left[ \mathsf{j} \right] \right) /. \; \mathsf{Rules2} \; / / \; \mathsf{Simplify}
 In[•]:=
                  (Coefficient[\Delta F_{j}[j], S_{j}] - (B_{ml}[j] + B_{mu}[j])) /. Rules2 // Simplify
                  \left(\mathsf{Coefficient}\left[\Delta\mathsf{F}^{\mathsf{I}}{}_{\mathsf{j}}\left[\mathsf{j}\right]\mathsf{,\,S}_{\mathsf{j}+1}\right]\;\mathsf{-\,B}_{\mathsf{upper}}\left[\mathsf{j}\right]\right)\;\mathsf{/\,.\,Rules2\;//\,Simplify}
                  (Coefficient \Delta F_1[[1]], S_1 - (B_{ml}[1] + B_{mu}[1]) /. Rules2 // Simplify
                  (Coefficient \Delta F_{N}[[1]], S_{N} - (B_{m1}[N] + B_{mu}[N]) /. Rules2 // Simplify
                 0
Out[•]=
                 0
Out[•]=
                 0
Out[•]=
                 0
Out[•]=
```

0

Out[•]=