KU LEUVEN

Project Mathematical Engineering

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Mathematical Engineering

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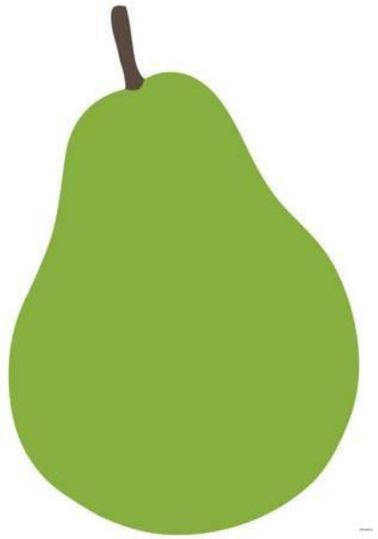
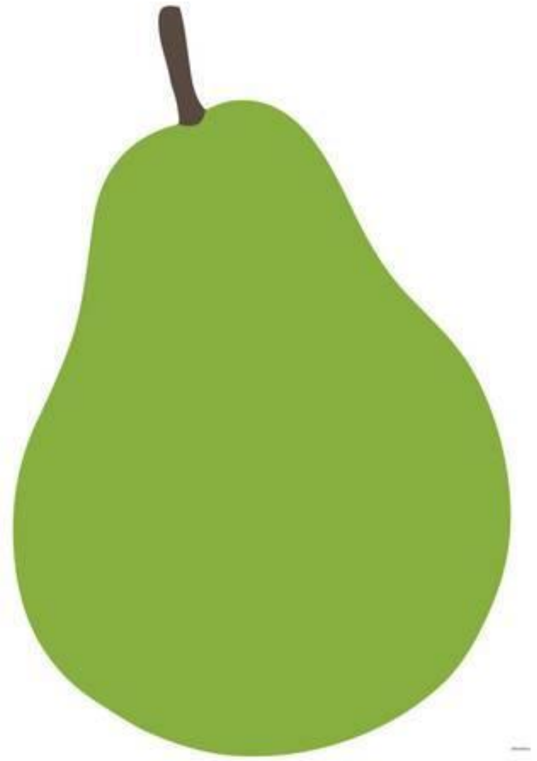
Pear Project: Contents



1. Mathematical Problem



- Challenge: Simulate and predict internal gas concentrations/ distributions

- Study the effect of controlled storage conditions on local oxygen and carbon dioxide concentrations

1. Mathematical Problem: Model

- **Model** used for system:
  - Non-linear **reaction-diffusion equations**: in stationary regime
  - On **two-dimensional bounded** spatial domain
  - u: oxygen   v:carbon-dioxide

$$\begin{cases} \nabla \cdot \left(r \begin{pmatrix} \sigma_{u,r} & 0 \\ 0 & \sigma_{u,z} \end{pmatrix} \nabla C_u(r,z) \right) = r\, R_u(C_u(r,z), C_v(r,z)) \\ \nabla \cdot \left(r \begin{pmatrix} \sigma_{v,r} & 0 \\ 0 & \sigma_{v,z} \end{pmatrix} \nabla C_v(r,z) \right) = -r\, R_v(C_u(r,z), C_v(r,z)) \end{cases} \quad \text{for} \quad (r,z) \in \Omega$$

1. Mathematical Problem: Boundary Conditions

- **Boundary Conditions**:
  - Internal Boundary: $(C_u^*(r,z), C_v^*(r,z)) = (0,0)$
  - External Boundary: $(C_u^*(r,z), C_v^*(r,z)) = (C_u(r,z) - C_{u\mathrm{amb}}, C_v(r,z) - C_{v\mathrm{amb}})$

Ambient concentrations

$$\begin{cases} -\vec{n}(r,z) \cdot \left(\begin{pmatrix} \sigma_{u,r} & 0 \\ 0 & \sigma_{u,z} \end{pmatrix} \nabla C_u(r,z) \right) = \varrho_u \, C_u^*(r,z) \\ -\vec{n}(r,z) \cdot \left(\begin{pmatrix} \sigma_{v,r} & 0 \\ 0 & \sigma_{v,z} \end{pmatrix} \nabla C_v(r,z) \right) = \varrho_v \, C_v^*(r,z) \end{cases} \quad \text{for} \quad (r,z) \in \Gamma,$$

1. Mathematical Problem: Respiration kinetics

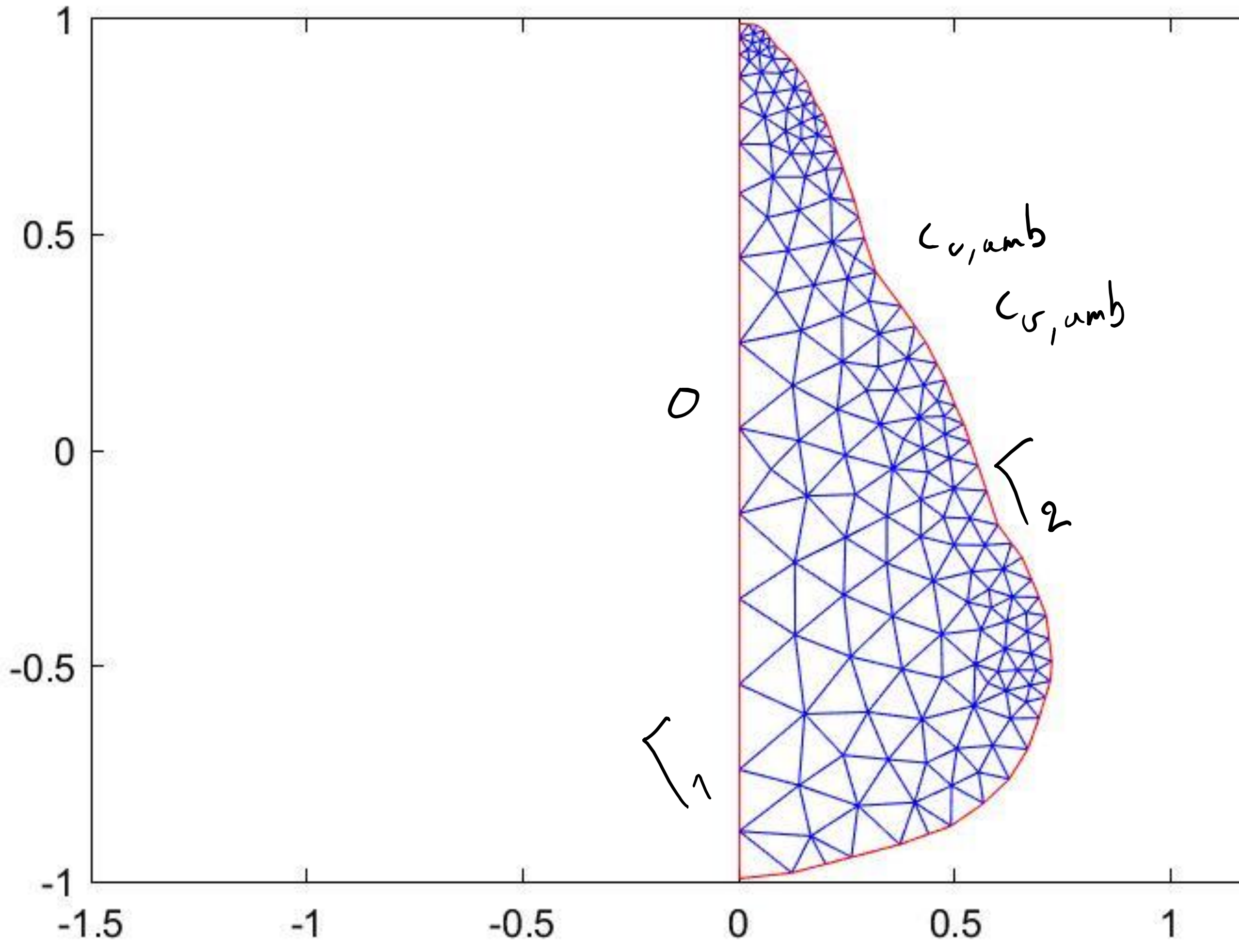
- **Respiration Kinetics:**

  Describe the **evolution** of the system through **gas exchange** with the environment

$$\begin{cases} R_u(C_u, C_v) = \dfrac{V_{mu} C_u}{(K_{mu} + C_u)\left(1 + \dfrac{C_v}{K_{mv}}\right)} \\ \\ R_v(C_u, C_v) = r_q\, R_u(C_u, C_v) + \dfrac{V_{mfv}}{1 + \dfrac{C_u}{K_{mfu}}} \end{cases}$$

2. Description of FE-method

- Domain is split up into triangles consisting of M nodes
- We want to approximate the solutions at the nodes of our mesh by use of linear basisfunctions
- In every triangle we use three basisfunctions to represent our solution.
- On every edge we use two basisfunctions to represent our solution.



2. Description of FE-method

$$\vec{q}_u(r,z) = r\begin{pmatrix}\sigma_{u,r} & 0\\ 0 & \sigma_{u,z}\end{pmatrix}\nabla C_u(r,z)$$

$$C_u^M(r,z) := \sum_{j=1}^{M} c_i\,\varphi_i(r,z),$$

$$\int_\Omega \vec{q}_u(r,z)\cdot\nabla\varphi(r,z)\,\mathrm{d}\Omega + \int_\Omega r\,R_u(C_u,C_v)\,\varphi(r,z)\,\mathrm{d}\Omega + \int_\Gamma r\,\varrho_u\,C_u^*(r,z)\,\varphi(r,z)\,\mathrm{d}\Gamma = 0$$

$$\begin{pmatrix}K_u & 0\\ 0 & K_v\end{pmatrix}\begin{pmatrix}\mathbf{c}_u\\ \mathbf{c}_v\end{pmatrix} - \begin{pmatrix}\mathbf{f}_u\\ \mathbf{f}_v\end{pmatrix} + \begin{pmatrix}\mathbf{H}_u(\mathbf{c}_u,\mathbf{c}_v)\\ \mathbf{H}_v(\mathbf{c}_u,\mathbf{c}_v)\end{pmatrix} = \begin{pmatrix}\mathbf{0}\\ \mathbf{0}\end{pmatrix}$$

Ω : Internal

Γ : Edge

We solve these integrals by looping over all triangles/edges. The integral becomes a sum of integrals.

2. Description of FE-method

$$\vec{q}_u(r,z) = r\begin{pmatrix}\sigma_{u,r} & 0\\ 0 & \sigma_{u,z}\end{pmatrix}\nabla C_u(r,z)$$

$$C_u^M(r,z) := \sum_{j=1}^{M} c_i\,\varphi_i(r,z),$$

- For example start from: $\displaystyle\int_\Omega \vec{q}_u(r,z)\cdot\nabla\varphi(r,z)\,\mathrm{d}\Omega$

- Each triangle is mapped onto standard triangle:

  with $r = x_1^T\widehat{N}_1 + x_2^T\widehat{N}_2 + x_3^T\widehat{N}_3$

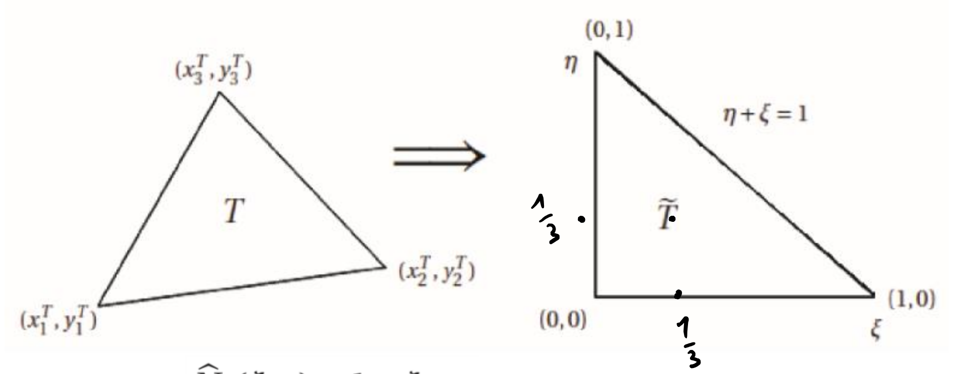
- With derivatives of basisfunctions in each triangle

  with: $|J| = \begin{vmatrix}\frac{\partial x}{\partial\xi} & \frac{\partial x}{\partial\eta}\\ \frac{\partial y}{\partial\xi} & \frac{\partial y}{\partial\eta}\end{vmatrix} = \begin{vmatrix}x_2^T - x_1^T & x_3^T - x_1^T\\ y_2^T - y_1^T & y_3^T - y_1^T\end{vmatrix}$

$$\frac{\partial N_1}{\partial x} = \frac{1}{|J|}(y_2^T - y_3^T) \qquad \frac{\partial N_1}{\partial y} = \frac{1}{|J|}(x_3^T - x_2^T)$$

$$\frac{\partial N_2}{\partial x} = \frac{1}{|J|}(y_3^T - y_1^T) \qquad \frac{\partial N_2}{\partial y} = -\frac{1}{|J|}(x_3^T - x_1^T)$$

$$\frac{\partial N_3}{\partial x} = -\frac{1}{|J|}(y_2^T - y_1^T) \qquad \frac{\partial N_3}{\partial y} = \frac{1}{|J|}(x_2^T - x_1^T)$$



$$\widehat{N}_1(\xi,\eta) = 1 - \xi - \eta$$

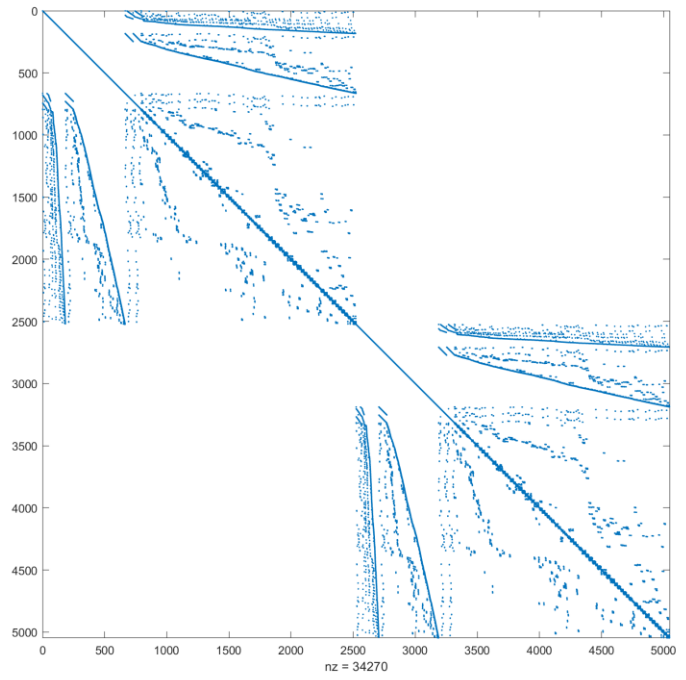
$$\widehat{N}_2(\xi,\eta) = \xi$$

$$\widehat{N}_3(\xi,\eta) = \eta$$

3. Construction of Linear System

- Using this technique we fill the matrix of the linear system (K):
  -> 9 adjustments (combinations of 3 nodes) are made to Ku and Kv for every triangle handled.

- Sparsity pattern is obtained:

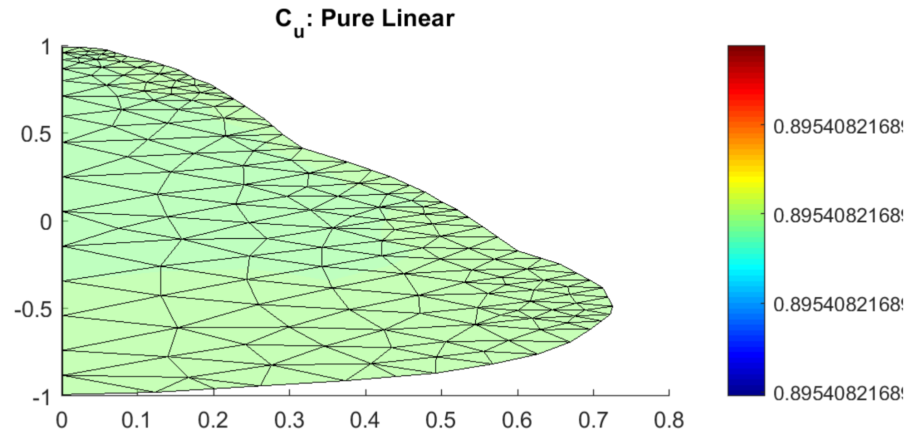


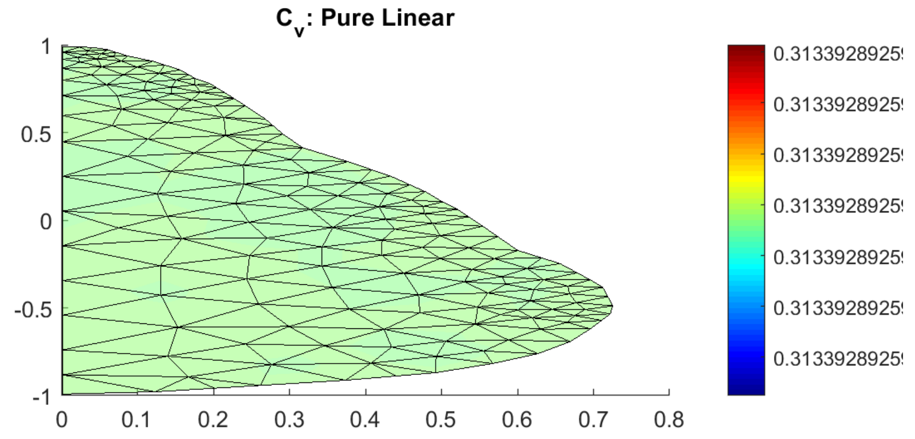
3. Demonstration of Result for Linear System

- Initial plots give expected result

->values near the ambient O2 and CO2 concentration

Figure generated with data from FORTRAN





3. Construction of Linear System

- Integral over edge: $$\int_{\Gamma \to \Gamma_2} r\,\varrho_u\,C_u^*(r,z)\,\varphi(r,z)\,\mathrm{d}\Gamma$$
- Map edge onto standard line
- Two basisfunctions instead of three: $r = x_1^T \widehat{N}_1 + x_2^T \widehat{N}_2$
- Integral for one edge translates to: $\int_0^1 r\,\varrho_u\,C_u^*(\xi,\eta)\,\hat{N}(\xi,\eta)\,d\xi$
- This integral can be computed (mupad)
- For every edge: two adjustments are made to Fu and Fv as well as to Ku and Kv
- If we now calculate   K*c = F (ignore H) then we find: c= [C_uamb…C_vamb…] (steady state)

$$\widehat{N}_1(\xi,\eta) = \xi$$
$$\widehat{N}_2(\xi,\eta) = 1 - \xi$$

3. Construction of Linear System: Linearization

- Goal: find initial values (c_u0,c_v0) to start newton iteration

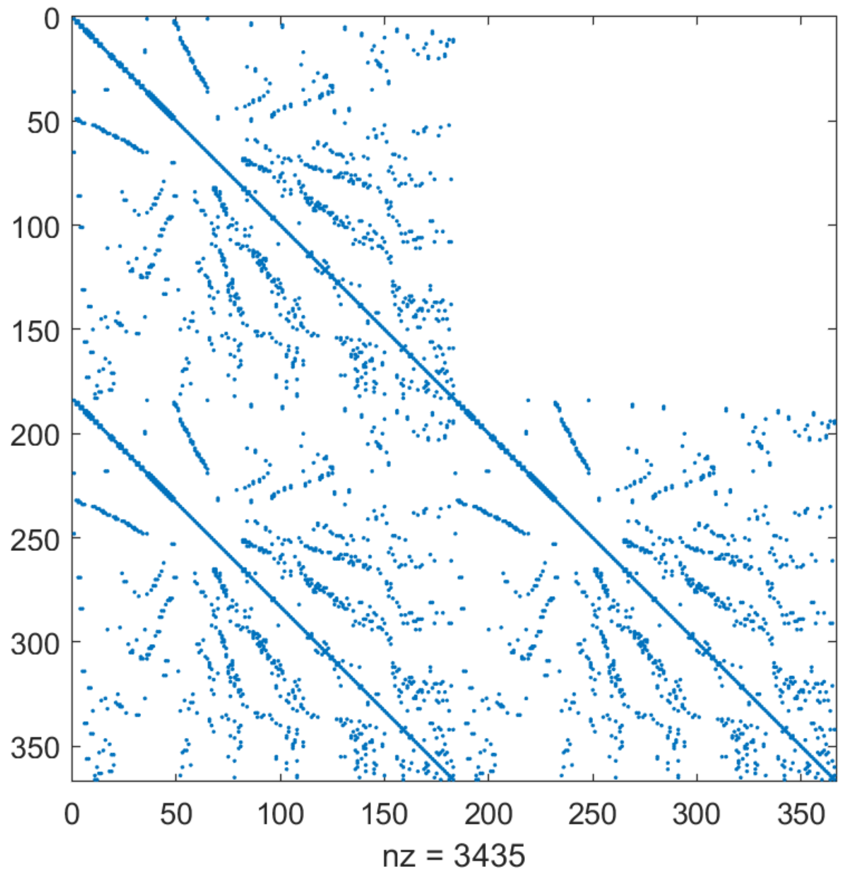
- Linearize H_u and H_v around Cu =0 (no oxygen within pear, because it is turned into CO2 really fast)
  -> This leads to a simple expression for R_u and R_v

- Contribution to the K-matrix and f-vector after which system can be solved again

3. Construction of Linear System: Linearization

- The linearization causes changes to the K-matrix; its form becomes:

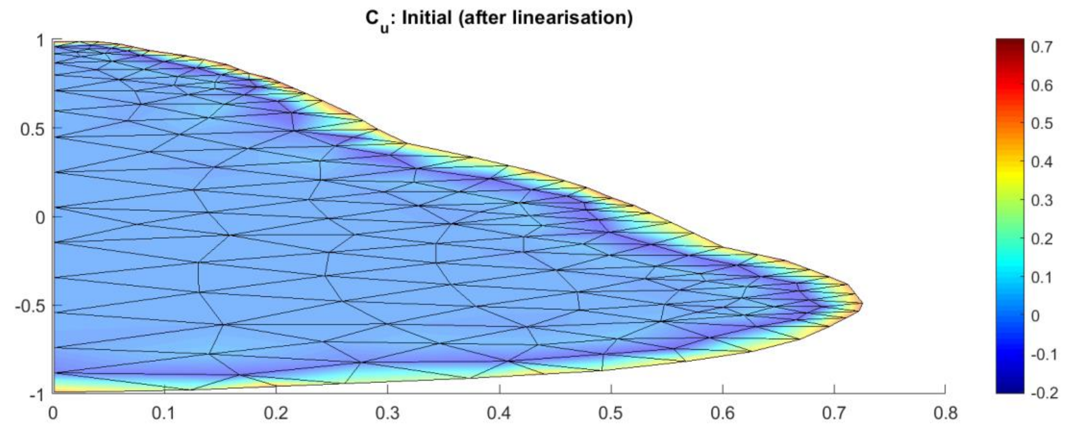
- Using this we can solve the linear system: c0 = K\f. In FORTRAN, this is solved by using a pivot-version of the Gauss algorithm.

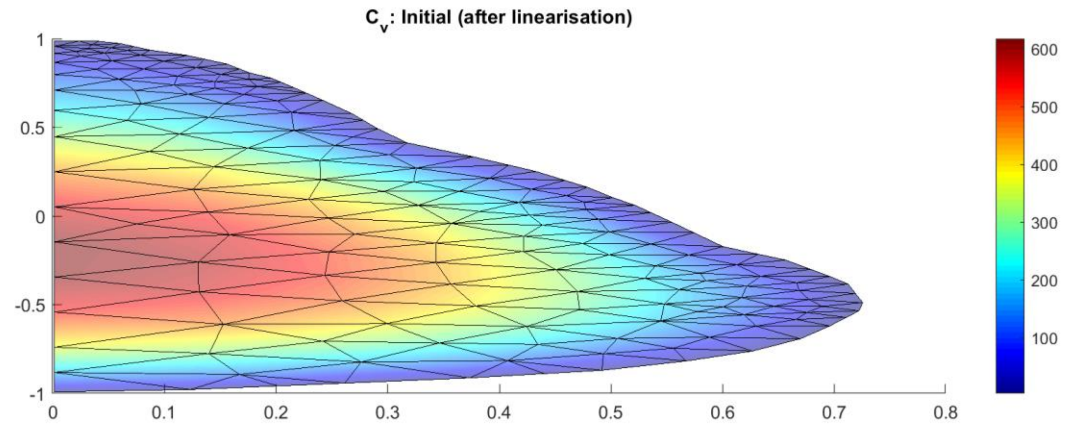


4. Results for initial values after linearisation

- Using FORTRAN and MATLAB we get the same results.
- Both concentrations show expected evolution pattern.
- O2 concentration distribution is too heavily concentrated near the edges

Figure generated with data from FORTRAN





5. Solving Nonlinear System

- We use the Newton-Raphson Iterative Algorithm

$$F(c_u, c_v) = \begin{pmatrix} K_u & 0 \\ 0 & K_v \end{pmatrix} \begin{pmatrix} \mathbf{c}_u \\ \mathbf{c}_v \end{pmatrix} - \begin{pmatrix} \mathbf{f}_u \\ \mathbf{f}_v \end{pmatrix} + \begin{pmatrix} \mathbf{H}_u(\mathbf{c}_u, \mathbf{c}_v) \\ \mathbf{H}_v(\mathbf{c}_u, \mathbf{c}_v) \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \end{pmatrix}$$

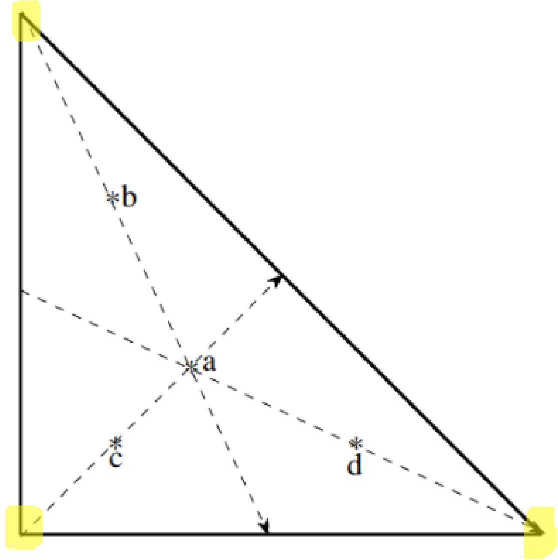
$$J(c_u, c_v) = \begin{bmatrix} K_u + \frac{\partial H_u}{\partial c_u} & \frac{\partial H_u}{\partial c_v} \\ \frac{\partial H_v}{\partial c_u} & K_v + \frac{\partial H_v}{\partial c_v} \end{bmatrix}$$

- $c_{k+1} = c_k - J^{-1}(c_k) \cdot F(c_k)$

5. Solving Nonlinear System

- Used Gaussian (degree 3 precision) quadrature formula to approximate integral

$$\iint_{T_{\mathrm{st}}} g(\xi,\eta)\,\mathrm{d}\xi\mathrm{d}\eta = -\frac{27}{96}\cdot g\left(\frac{1}{3},\frac{1}{3}\right) + \frac{25}{96}\left[g\left(\frac{1}{5},\frac{1}{5}\right) + g\left(\frac{1}{5},\frac{3}{5}\right) + g\left(\frac{3}{5},\frac{1}{5}\right)\right]$$



$$C_u = C_{u_1}(1-\xi-\eta) + C_{u_2}\xi + C_{u_3}\eta$$

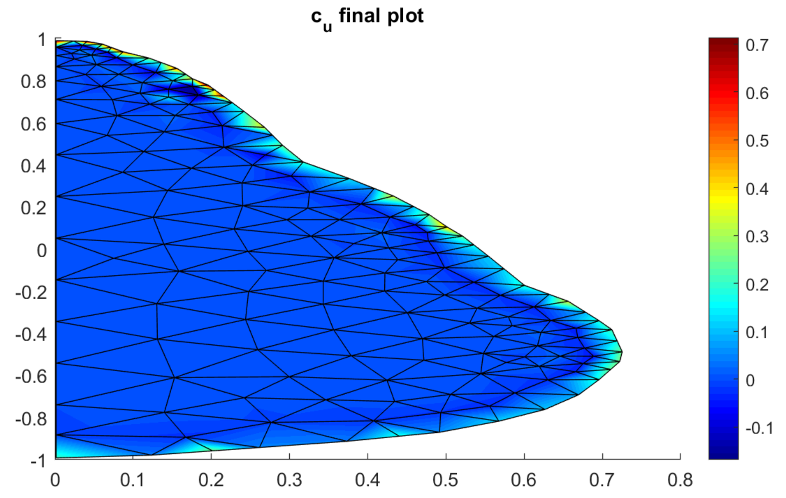
$$C_v = C_{v_1}(1-\xi-\eta) + C_{v_2}\xi + C_{v_3}\eta$$

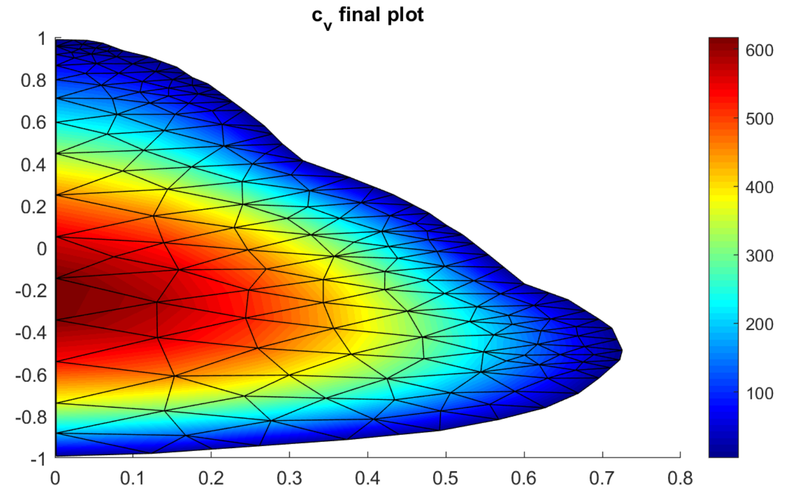
🟨 = known values in vertices from previous iteration

6. Demonstration of results of nonlinear problem

- In FORTRAN: used MINPACK library to solve nonlinear system of equations (jacobian approximated by forward diffenrences)
- In MATLAB: Calculated Jacobian analytically, result checked by calculating via finite differences function
- The distribution of the CO2 concentration is as we would expect it.
- The distribution of the O2 has not changed much from the initial values.

Figure generated with data from MATLAB





Timing comparison: Fortran vs Matlab

- Using a maximum of 100 iterations for both ways of solving the non-linear system, we got following timings for the same pear:
  - FORTRAN: 0.3948s (average)
  - MATLAB: 5.3906s (average)

Conclusion

- Problems:
  - Not completly correct initial concentration (linearisation assumptions?)
  - Convergence to wrong solutions when solving non-linear system

- Insights
  - More detailed understanding of Finite Element Method
  - Use of quadrature rules in practice
  - Structured MATLAB-programming
  - Structured FORTRAN-programming and working with library (MINPACK)
  - FORTRAN is much faster than MATLAB (also because of efficient solver)