

ME40064 System Modelling and Simulation - Coursework 2

1252 Words, Candidate No. 11973, 2nd December 2025

Department of Mechanical Engineering, University of Bath

1. Introduction

Finite Element Method (FEM) is a powerful numerical technique for solving equations over a discrete domain. The simulated system is split into small regions called **elements**, connected by **nodes** which represent discrete points in the domain, together making up a **mesh**. Elements are evaluated using **basis functions** which approximate the solution within each element based on node values [1]. This approach allows for practical solutions to problems that may be difficult or impossible to solve analytically. In addition to this, the size and shape of elements can be adjusted to improve accuracy or reduce computational cost, making FEM a powerful and flexible tool for modelling (Figure 1).

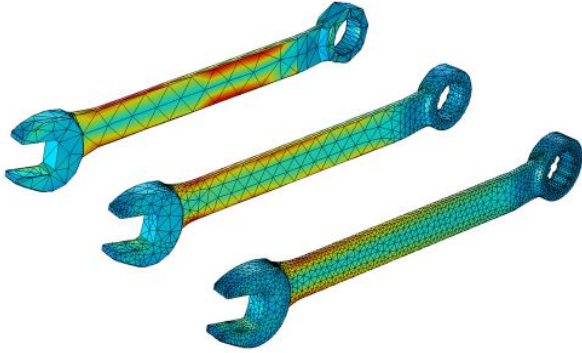


Figure 1: Finite Element Modelling of a Wrench under a Test Load Scenario [2]

This coursework focuses on the implementation and verification of a FEM solver for the transient diffusion-reaction equation, given by [3]:

$$\frac{\delta c}{\delta t} = D \frac{\delta^2 c}{\delta x^2} + \lambda c + f \quad (1)$$

Where:

- c is the concentration level
- D is the diffusion coefficient
- λ is the reaction rate
- f is a source term

The transient diffusion-reaction equation models processes where substances diffuse through a medium while undergoing reactions or being influenced by boundary interactions. Examples of situations modelled by this equation include the transfer of heat through a material or (as explored in Part 3 of this report) the diffusion of a drug through biological tissue.

This coursework describes the development and validation of a FEM solver for the transient diffusion-reaction equation. To keep the scope manageable, the solver was implemented in 1D, using MATLAB as the scripting language [4].

2. Part 1: Software Verification

2.1. Background

A static FEM solver was implemented in a previous coursework for the steady-state diffusion-reaction equation. This solver was subsequently adapted to solve the transient form of the equation (Equation 1).

For the initial case, the values of $D = 1$ and $\lambda = 0$ were used, representing a pure diffusion scenario with linear behaviour. The **Crank-Nicolson** finite difference method was used for time integration. It has unconditional stability but no damping of oscillations, providing a good compromise between accuracy and stability at this stage [5].

The problem space was further defined with the following conditions:

Problem Space	$0 \leq x \leq 1$
Left Boundary Condition	Dirichlet: $c(0, t) = 0$
Right Boundary Condition	Dirichlet: $c(1, t) = 1$
Initial Condition	$c(x, 0) = 0$

Table 1: Initial Case Conditions

These conditions have a known analytical solution, given by Equation 2:

$$c(x, t) = x + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^n}{n} e^{-n^2 \pi^2 t} \sin(n \pi x) \quad (2)$$

The analytical solution allows for direct comparison of results between the FEM solver and expected values, providing a quantitative measure of accuracy.

2.2. Software Architecture

The solver was implemented with a modular, object-oriented software architecture to improve readability and control flow. Classes were created to encapsulate well-defined functions of the solver, such as mesh generation or plotting (Figure 2).

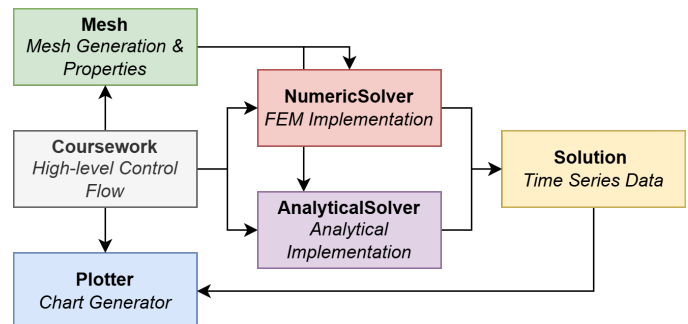


Figure 2: High-Level Software Architecture of the FEM Solver

2.3. Results

Having implemented the FEM solver as described above, a simulation was run using a mesh size of 50 elements and a time step of 0.01s, over the time period $0 < t \leq 1s$.

After this, the results were plotted on a series of charts for a visual comparison of the two solutions. The first of these were heatmaps which are an effective method for visualising the 1D diffusion over time (Figure 4, Figure 3).

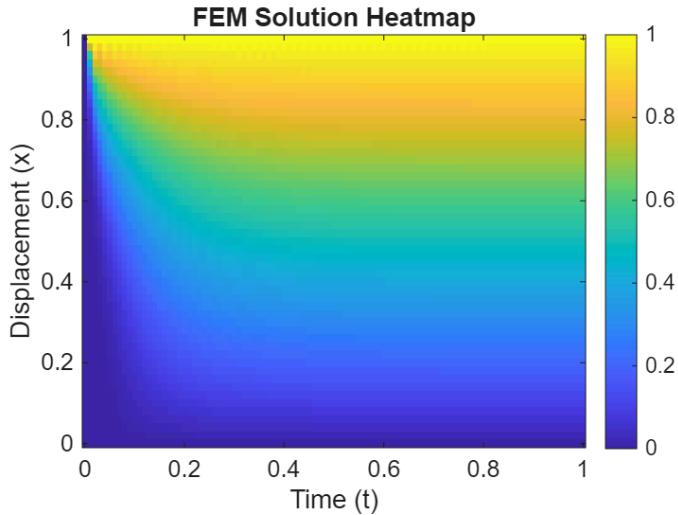


Figure 3: FEM Solution of Diffusion Equation over using the Crank-Nicolson method over $0 \leq x \leq 1$ and $0 \leq t \leq 1s$

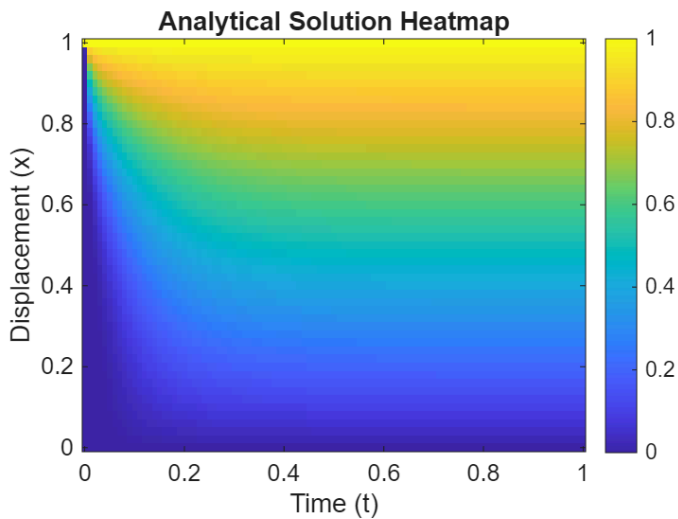


Figure 4: Analytical Solution of Diffusion Equation over $0 \leq x \leq 1$ and $0 \leq t \leq 1s$

The data was also represented in a 2D plot, showing the concentration through the mesh at sample times of $t = 0.05s, 0.1s, 0.3s, 1.0s$, shown in Figure 5 and Figure 6.

Additionally, a chart was created for both solutions at a single point in the mesh ($x = 0.8$), shown in Figure 7. Unlike previous plots, this shows both methods on the same axes for direct comparison, demonstrating the agreement between the two solutions.

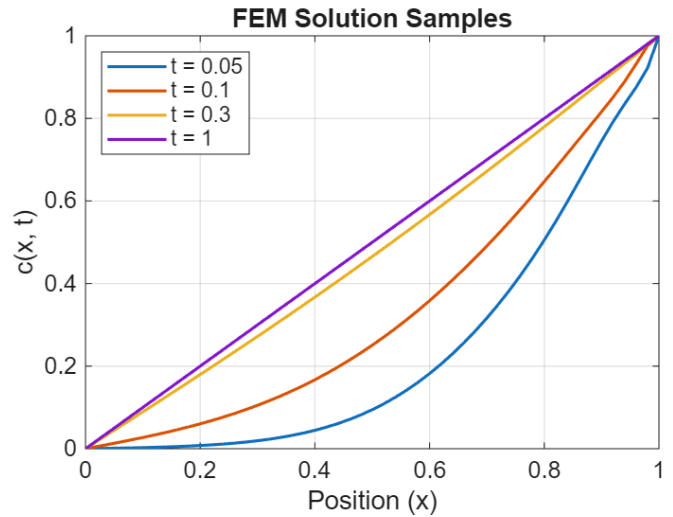


Figure 5: FEM Solution of Diffusion Equation over using the Crank-Nicolson method over $0 \leq x \leq 1$ and at $t = 0.05s, 0.1s, 0.3s, 1.0s$

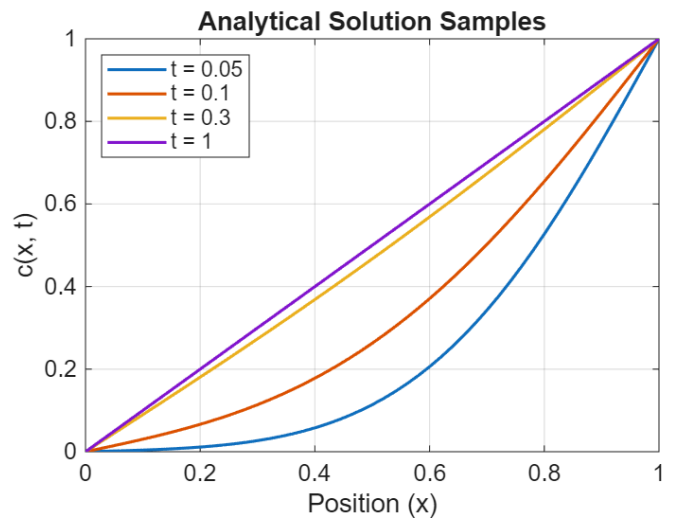


Figure 6: Analytical Solution of Diffusion Equation over $0 \leq x \leq 1$ and at $t = 0.05s, 0.1s, 0.3s, 1.0s$

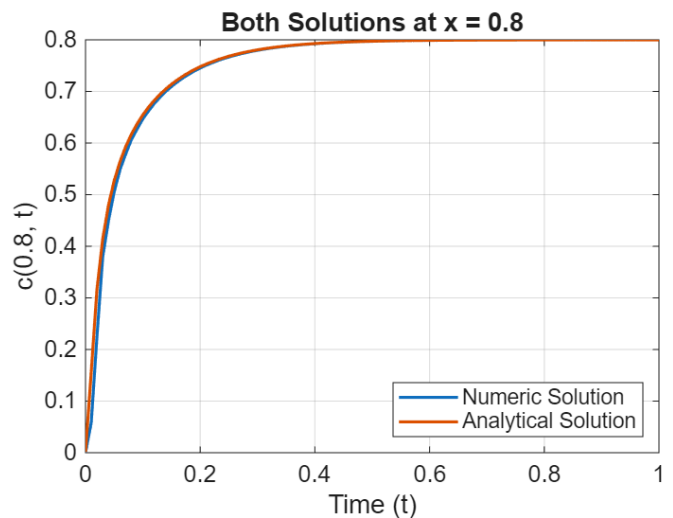


Figure 7: Comparison of Analytical and FEM Solutions at $x = 0.8$ over $0 \leq t \leq 1s$

2.4. Spacial and Temporal Convergence

To quantitatively assess the accuracy of the FEM solver, the **Root Mean Square (RMS)** error between numerical and analytical solutions was evaluated over a range of element and time step sizes. As shown in Figure 8 and Figure 9, the RMS error decreases with both smaller element sizes and smaller time steps, demonstrating convergence of the numerical solution towards the analytical solution with increasing resolution.

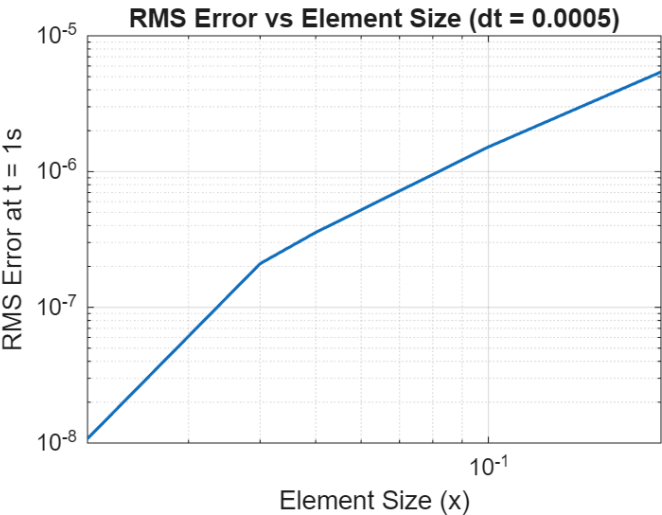


Figure 8: Comparison of RMS errors at $t = 1s$ for Varying Element Sizes

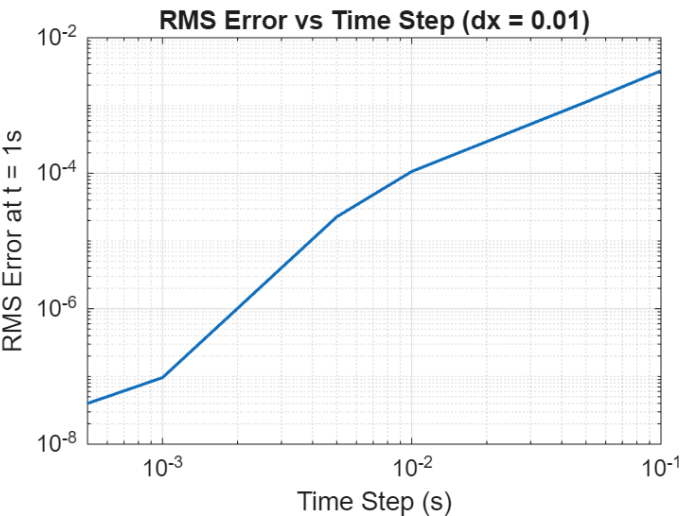


Figure 9: Comparison of RMS errors at $t = 1s$ for Varying Time Steps

2.5. Testing and Validation

A set of unit tests were created alongside the FEM solver, to verify the functionality of individual components such as mesh generation, element assembly, and time integration. As part of the development process, the project was continuously tested to ensure it passed all scenarios.

In particular, a unit test was created to validate the solver against a manufactured solution of the transient diffusion-reaction equation. This involved selecting specific values for D , λ , and f such that the solution could be expressed in a simple analytical form.

3. Part 2: Software features

3.1. Error Evaluation

In Part 1 of the coursework, the RMS error term was used to evaluate the accuracy of the FEM solver. While RMS is a useful metric, it can be sensitive to outliers and therefore may not always provide a complete picture of the solution accuracy. L2 norm doesn't suffer as much from this, and is more widely used in literature as a result [3]. To address this, a dedicated L2 error evaluation class was added to the solver, allowing for more robust error analysis.

3.2. Integration Methods

Using the L2 norm error evaluation class, the performance of three different time integration methods was compared: Forward (Explicit) Euler, Backward (Implicit) Euler, and Crank-Nicolson. This test was run using a mesh with 10 elements and a time step size of 0.0001s.

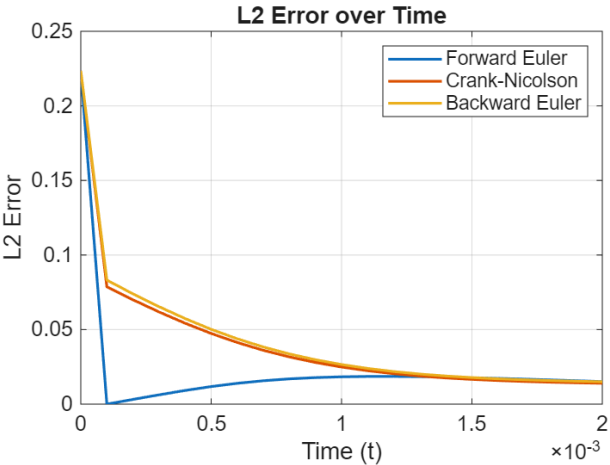


Figure 10: Comparison of L2 Errors for Different Time Integration Methods

This shows that the Forward Euler method had a higher initial accuracy, approaching the solution more quickly than the other two methods, but that it started to decrease in accuracy again afterwards. This was likely caused by instability in the method, as it is only conditionally stable.

To illustrate this further, a stability analysis was performed for all three methods, using a larger mesh of 50 elements:

dt	Forward Euler	Backward Euler	Crank-Nicolson
0.0001	Stable	Stable	Stable
0.001	Unstable	Stable	Stable
0.01	Unstable	Stable	Stable
0.1	Unstable	Stable	Stable
0.25	Unstable	Stable	Stable

Table 2: Integration Method Stability Comparison

This shows that the Forward Euler method was only stable for very small time steps, while the other two methods demonstrated **unconditional stability**, remaining stable across all tested time steps.

For linear finite elements, the stability condition for the Forward Euler method is given by the following equation [6]:

$$dt \leq \frac{dx^2}{2D} \quad (3)$$

Therefore, for a mesh with 50 elements over the domain $0 \leq x \leq 1$ and $D = 1$, the value of dt must be no more than 0.0002s for stability, which aligns with the results shown in Table 2.

3.3. Gaussian Quadrature

So far, the solver has only been used with a simple 2-point trapezoidal integration method for evaluating element matrices. While this method is easy to implement, it treats all elements as linear, requiring meshes with high numbers of elements to achieve good accuracy for non-linear problems.

Gaussian Quadrature is an alternative integration method that can provide a more accurate result with the same number of integration points as trapezoidal integration, resulting in a more efficient solution [7].

3.4. Quadratic Basis Functions

For 2-point basis functions like those used in the coursework so far, Gaussian Quadrature with 2 points will produce an identical result to trapezoidal integration. The mesh was therefore updated to support higher-order basis functions, such as quadratic (3-point) elements, where each element has a node at each end and one in the middle.

The L2 error of a quadratic mesh with both trapezoidal and Gaussian integration methods is shown below in Figure 11:

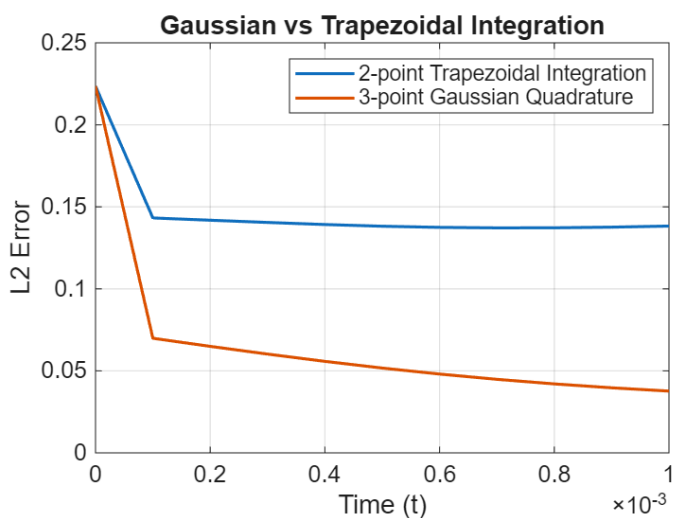


Figure 11: Comparison of L2 Errors for Gaussian Quadrature and Trapezoidal Integration

This shows a clear improvement in accuracy when using Gaussian Quadrature over trapezoidal integration with quadratic basis functions, approaching the analytical solution in a shorter time.

3.5. Summary of Features

The addition of L2 error evaluation was an effective way to quantitatively assess the accuracy of the FEM solver, with varying configurations. It was found that the Crank-Nicolson method remained a suitable choice for time integration, balancing accuracy and stability, while the addition of Gaussian Quadrature and higher-order basis functions showed a significant improvement to solution accuracy.

4. Part 3: Modelling & Simulation Results

4.1. Mesh Refining

NEED TO REFINE MESH!

5. Conclusion

6. References

- [1] J. L. G. Dhatt G. Touzot, *Finite Element Method*. Wiley.
- [2] "Finite Element Mesh Refinement." [Online]. Available: <https://www.comsol.com/multiphysics/mesh-refinement>
- [3] W. Hundsdorfer, "Numerical Solution of Advection-Diffusion-Reaction Equations," 2000. [Online]. Available: <https://bpb-us-e1.wpmucdn.com/blogs.gwu.edu/dist/9/297/files/2018/01/66bdd115ac105ea17af303e73d4fec449754-v448bk.pdf>
- [4] "MATLAB." [Online]. Available: <https://mathworks.com/products/matlab.html>
- [5] C. W. T. C. Sun, "Unconditionally stable Crank-Nicolson scheme for solving two-dimensional Maxwell's equations," 2003. [Online]. Available: <https://doi.org/10.1049/el:20030416>
- [6] C. Connaughton, "The Diffusion Equation," 2009. [Online]. Available: https://warwick.ac.uk/fac/cross_fac/complexity/study/msc_and_phd/co906/co906online/lecturenotes_2009/chap3.pdf
- [7] T. Amisaki, "Gaussian Quadrature as a Numerical Integration Method for Estimating Area Under the Curve," 2001. [Online]. Available: https://www.jstage.jst.go.jp/article/bpb/24/1/24_1_70/_pdf/-char/ja

7. Use of Generative AI

This coursework was completed in Visual Studio Code (with the MATLAB Extension), using Typst for report

writing. The [GitHub Copilot](#) AI tool was enabled, providing generative suggestions for report phrasing and code snippets.

8. Appendix - MATLAB Source Code

9. Main

9.1. main.m

```
1 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
2 %
3 % ME40064 Coursework 2
4 %
5 % File      : main.m
6 % Author    : samh25
7 % Created   : 2025-11-24 (YYYY-MM-DD)
8 % License   : MIT
9 % Description : Main function for solving transient diffusion equation
10 %
11 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
12
13 function main()
14     fprintf("ME40064 Coursework 2 Starting...\n");
15
16     Coursework.Part2GaussianQuadrature();
17
18     fprintf("...ME40064 Coursework 2 Complete\n");
19 end
20
```

10. Coursework

10.1. Coursework.m

```

1 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
2 %
3 % ME40064 Coursework 2
4 %
5 % File      : Coursework.m
6 % Author    : samh25
7 % Created   : 2025-11-27 (YYYY-MM-DD)
8 % License   : MIT
9 % Description : Static methods for each part of the coursework.
10 %
11 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
12
13 classdef Coursework
14
15     methods (Static)
16
17         function Part1Plots()
18             %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
19             %
20             % Function:      Part1Plots()
21             %
22             % Arguments:     None
23             % Returns:       None
24             %
25             % Description:   Runs the start Part 1 of the coursework,
26                             % generating a simple mesh, running numeric and
27                             % analytical solvers, and plotting the results.
28             %
29             %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
30
31             % time parameters
32             tmax = 1.0;
33             dt = 0.01;
34
35             % mesh parameters
36             xmin = 0.0;
37             xmax = 1.0;
38             element_count = 50;
39             order = 1;
40
41             % Crank-Nicholson method
42             theta = 0.5;
43
44             % diffusion and reaction coefficients
45             D = 1.0;
46             lambda = 0.0;
47
48             % concentrations
49             c_max = 1.0;
50             c_min = 0.0;
51
52
53             % generate mesh
54             mesh = Mesh(xmin, xmax, element_count, order, D, lambda);
55             mesh.Generate();
56
57             % solver parameters
58             lhs_boundary = BoundaryCondition();
59             lhs_boundary.Type = BoundaryType.Dirichlet;
60             lhs_boundary.Value = c_min;
61
62             rhs_boundary = BoundaryCondition();
63             rhs_boundary.Type = BoundaryType.Dirichlet;

```



```

64         rhs_boundary.Value = c_max;
65
66         integration_method = IntegrationMethod();
67         integration_method.type = IntegrationType.Trapezoidal;
68         integration_method.gauss_points = 0; % not used for trapezoidal
69
70         % solve numerically
71         numeric_solution = NumericSolver.SolveNumeric(...
72             mesh, tmax, dt, theta, lhs_boundary, rhs_boundary, @(~, ~) 0.0,
integration_method);
73
74         % solve analytically
75         analytical_solution = AnalyticalSolver.SolveAnalytical(mesh, tmax, dt);
76
77         % plot solutions as heatmaps
78         Plotter.PlotHeatMap(numeric_solution, "FEM Solution Heatmap", ...
79             "cw2/report/resources/part1/NumericHeatmap", c_max);
80         Plotter.PlotHeatMap(analytical_solution, "Analytical Solution Heatmap", ...
81             "cw2/report/resources/part1/AnalyticalHeatmap", c_max);
82
83         % plot solution samples at specified times
84         sample_times = [0.05, 0.1, 0.3, 1.0];
85         Plotter.PlotTimeSamples(numeric_solution, dt, sample_times, "FEM Solution
Samples", ...
86             "cw2/report/resources/part1/NumericSamples");
87         Plotter.PlotTimeSamples(analytical_solution, dt, sample_times, "Analytical
Solution Samples", ...
88             "cw2/report/resources/part1/AnalyticalSamples");
89
90         % plot both solutions at a specific position over time
91         sample_x = 0.8;
92         legend_strings = {"Numeric Solution", "Analytical Solution"};
93         Plotter.PlotSampleOverTime(numeric_solution, analytical_solution, ...
94             sample_x, "Both Solutions at x = 0.8", "cw2/report/resources/part1/
BothX08", legend_strings);
95
96     end
97
98     function Part1Convergence()
99         %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
100        %
101        % Function:      Part1Convergence()
102        %
103        % Arguments:    None
104        % Returns:      None
105        %
106        % Description:  Runs a convergence study for Part 1 of the
107        %               coursework, calculating RMS error between numeric
108        %               and analytical solutions over a range of element
109        %               counts and time steps.
110        %
111        %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
112
113        % time parameters
114        tmax = 1.0;
115
116        % mesh parameters
117        xmin = 0.0;
118        xmax = 1.0;
119        element_count = 50;
120        order = 1;
121
122        % Crank-Nicholson method
123        theta = 0.5;
124
125        % diffusion and reaction coefficients
126        D = 1.0;

```



```

127         lambda = 0.0;
128
129         % concentrations
130         c_max = 1.0;
131         c_min = 0.0;
132
133
134         % generate mesh
135         mesh = Mesh(xmin, xmax, element_count, order, D, lambda);
136         mesh.Generate();
137
138         % solver parameters
139         lhs_boundary = BoundaryCondition();
140         lhs_boundary.Type = BoundaryType.Dirichlet;
141         lhs_boundary.Value = c_min;
142
143         rhs_boundary = BoundaryCondition();
144         rhs_boundary.Type = BoundaryType.Dirichlet;
145         rhs_boundary.Value = c_max;
146
147         integration_method = IntegrationMethod();
148         integration_method.type = IntegrationType.Trapezoidal;
149         integration_method.gauss_points = 0; % not used for trapezoidal
150
151         % calculate RMS error with varying mesh sizes and time steps
152
153         element_counts = [5, 10, 20, 25, 50];
154         time_steps = [0.1, 0.05, 0.01, 0.005, 0.001, 0.0005];
155
156         num_cases = length(element_counts) * length(time_steps);
157         rms_errr_table_elem_count = zeros(num_cases, 4); % columns: elem_count, dt,
dx, RMS error
158         rms_errr_table_time_step = zeros(num_cases, 4); % columns: elem_count, dt,
dx, RMS error
159
160         k = 1;
161
162         % vary element count with fixed time step
163         for i = 1:length(element_counts)
164             elem_count = element_counts(i);
165             dt = 0.0005;
166
167             % generate mesh
168             mesh = Mesh(xmin, xmax, elem_count, order, D, lambda);
169             mesh.Generate();
170
171             % solve numerically
172             numeric_solution = NumericSolver.SolveNumeric(...
173                 mesh, tmax, dt, theta, lhs_boundary, rhs_boundary, @(~, ~) 0.0,
integration_method);
174
175             % solve analytically
176             analytical_solution = AnalyticalSolver.SolveAnalytical(mesh, tmax, dt);
177
178             % compute RMS error
179             [~, final_time] = min(abs(analytical_solution.time - tmax));
180
181             c_numeric = numeric_solution.values(:, final_time);
182             c_analytical = analytical_solution.values(:, final_time);
183
184             error = c_numeric - c_analytical;
185             rms_error = sqrt(mean(error.^2));
186
187             rms_errr_table_elem_count(k,:) = [elem_count, dt, (xmax-xmin)/elem_count,
rms_error];
188
189             k = k + 1;

```

```

190         fprintf("Elements: %d, dt: %.4f, dx: %.4f, RMS Error: %.6f\n", ...
191                 elem_count, dt, (xmax-xmin)/elem_count, rms_error);
192     end
193
194     k = 1;
195
196     % vary time step with fixed element count
197     for j = 1:length(time_steps)
198
199         elem_count = 1 / 0.01;
200         dt = time_steps(j);
201
202         % generate mesh
203         mesh = Mesh(xmin, xmax, elem_count, order, D, lambda);
204         mesh.Generate();
205
206         % solve numerically
207         numeric_solution = NumericSolver.SolveNumeric(...
208             mesh, tmax, dt, theta, lhs_boundary, rhs_boundary, @(~, ~) 0.0,
integration_method);
209
210         % solve analytically
211         analytical_solution = AnalyticalSolver.SolveAnalytical(mesh, tmax, dt);
212
213         % compute RMS error
214         [~, final_time] = min(abs(analytical_solution.time - tmax));
215
216         c_numeric = numeric_solution.values(:, final_time);
217         c_analytical = analytical_solution.values(:, final_time);
218
219         error = c_numeric - c_analytical;
220         rms_error = sqrt(mean(error.^2));
221
222         rms_errr_table_time_step(k,:) = [elem_count, dt, (xmax-xmin)/elem_count,
rms_error];
223
224         k = k + 1;
225
226         fprintf("Elements: %d, dt: %.4f, dx: %.4f, RMS Error: %.6f\n", ...
227                 elem_count, dt, (xmax-xmin)/elem_count, rms_error);
228     end
229
230     % plot element counts
231     dx = rms_errr_table_elem_count(:, 3); % element size
232     err_spatial = rms_errr_table_elem_count(:, 4);
233
234     Plotter.PlotConvergenceError(dx, err_spatial, ...
235         "RMS Error vs Element Size (dt = 0.0005)", ...
236         "cw2/report/resources/part1/ElementSizeConvergence", "Element Size (x)",
"RMS Error at t = 1s");
237
238     % plot time steps
239     dt_vals = rms_errr_table_time_step(:, 2); % time steps
240     err_temporal = rms_errr_table_time_step(:, 4);
241
242     Plotter.PlotConvergenceError(dt_vals, err_temporal, ...
243         "RMS Error vs Time Step (dx = 0.01)", ...
244         "cw2/report/resources/part1/TimeStepConvergence", "Time Step (s)", "RMS
Error at t = 1s");
245     end
246
247     function Part2TimeIntegrationComparison()
248     %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
249     %
250     % Function:      Part2TimeIntegrationComparison()
251     %
252     % Arguments:     None

```

```

253      % Returns:      None
254      %
255      % Description:  Runs a study comparing different time integration
256      %               methods for Part 2 of the coursework.
257      %
258      %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
259
260      % time parameters
261      tmax = 0.002;
262      dt = 0.0001;
263
264      % mesh parameters
265      xmin = 0.0;
266      xmax = 1.0;
267      element_count = 10;
268      order = 1;
269
270      % diffusion and reaction coefficients
271      D = 1.0;
272      lambda = 0.0;
273
274      % concentrations
275      c_max = 1.0;
276      c_min = 0.0;
277
278      % generate mesh
279      mesh = Mesh(xmin, xmax, element_count, order, D, lambda);
280      mesh.Generate();
281
282      % solve analytically
283      analytical_solution = AnalyticalSolver.SolveAnalytical(mesh, tmax, dt);
284
285      % solver parameters
286      lhs_boundary = BoundaryCondition();
287      lhs_boundary.Type = BoundaryType.Dirichlet;
288      lhs_boundary.Value = c_min;
289
290      rhs_boundary = BoundaryCondition();
291      rhs_boundary.Type = BoundaryType.Dirichlet;
292      rhs_boundary.Value = c_max;
293
294      integration_method = IntegrationMethod();
295      integration_method.type = IntegrationType.Trapezoidal;
296      integration_method.gauss_points = 0; % not used for trapezoidal
297
298
299      l2_errors = [];
300
301      thetas = [0.0, 1.0, 0.5]; % Explicit Euler, Implicit Euler, Crank-Nicholson
302      method_names = {"Forward Euler", "Crank-Nicolson", "Backward Euler"};
303
304      for i = 1:length(thetas)
305          theta = thetas(i);
306
307          % solve numerically
308          numeric_solution = NumericSolver.SolveNumeric(...
309              mesh, tmax, dt, theta, lhs_boundary, rhs_boundary, @(~, ~) 0.0,
310              integration_method);
311
312          % compute L2 error
313          l2_error = L2Error(analytical_solution, numeric_solution);
314          l2_errors = [l2_errors, l2_error];
315      end
316
317      Plotter.PlotL2Errors(l2_errors, "L2 Error over Time", ...
318          "cw2/report/resources/part2/L2ErrorTimeIntegration", ...
319          method_names);

```

```

319
320     % perform stability analysis
321
322     tmax = 1.0;
323     element_count = 50;
324     dt_list = [0.0001, 0.001, 0.01, 0.1, 0.25];
325
326     % generate mesh
327     mesh = Mesh(xmin, xmax, element_count, order, D, lambda);
328     mesh.Generate();
329
330     l2_errors_stability = [];
331
332     for i = 1:length(thetas)
333         theta = thetas(i);
334
335         l2_errors_dt = [];
336
337         for j = 1:length(dt_list)
338             dt = dt_list(j);
339
340             try
341
342                 fprintf("Testing %s with dt = %.4f...\n", method_names{i}, dt);
343
344                 numeric_solution = NumericSolver.SolveNumeric(...
345                     mesh, tmax, dt, theta, lhs_boundary, rhs_boundary, @(~, ~) 0.0,
integration_method);
346
347                 % CHECK FOR NaN/Inf at each timestep
348                 for t_idx = 1:length(numeric_solution.time)
349                     vals = numeric_solution.values(:, t_idx);
350                     if any(isnan(vals))
351                         fprintf("%s: NaN at step %d (t=%.4f)\n", method_names{i},
t_idx, numeric_solution.time(t_idx));
352                         break;
353                     end
354                     if any(isinf(vals))
355                         fprintf("%s: Inf at step %d (t=%.4f)\n", method_names{i},
t_idx, numeric_solution.time(t_idx));
356                         break;
357                     end
358
359                     if max(abs(vals)) > 1e10
360                         fprintf("%s: Explosion at step %d (t=%.4f), max=%.2e\n",
method_names{i}, t_idx, numeric_solution.time(t_idx), max(abs(vals)));
361                         break;
362                     end
363                 end
364
365                 analytical_solution = AnalyticalSolver.SolveAnalytical(mesh, tmax,
dt);
366
367                 l2_error = L2Error(analytical_solution, numeric_solution);
368
369                 l2_errors_dt = [l2_errors_dt, l2_error];
370             catch
371                 l2_errors_dt = [l2_errors_dt, NaN];
372                 fprintf("%s EXPLODED \n", method_names{i});
373             end
374         end
375
376         l2_errors_stability = [l2_errors_stability; l2_errors_dt];
377     end
378
379 end
380

```

```

381     function Part2GaussianQuadrature()
382     %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
383     %
384     % Function:      Part2GaussianQuadrature()
385     %
386     % Arguments:     None
387     % Returns:       None
388     %
389     % Description:   Runs a study comparing L2 error with and without
390     %               Gaussian Quadrature.
391     %
392     %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
393
394
395     % time parameters
396     tmax = 0.001;
397     dt = 0.0001;
398
399     % mesh parameters
400     xmin = 0.0;
401     xmax = 1.0;
402     element_count = 5;
403     order = 2;
404
405     % diffusion and reaction coefficients
406     D = 0.5;
407     lambda = 0.0;
408
409     % concentrations
410     c_max = 1.0;
411     c_min = 0.0;
412
413     % generate mesh
414     mesh = Mesh(xmin, xmax, element_count, order, D, lambda);
415     mesh.Generate();
416
417     % solve analytically
418     analytical_solution = AnalyticalSolver.SolveAnalytical(mesh, tmax, dt);
419
420     % solver parameters
421
422     theta = 0.5; % Crank-Nicholson
423
424     lhs_boundary = BoundaryCondition();
425     lhs_boundary.Type = BoundaryType.Dirichlet;
426     lhs_boundary.Value = c_min;
427
428     rhs_boundary = BoundaryCondition();
429     rhs_boundary.Type = BoundaryType.Dirichlet;
430     rhs_boundary.Value = c_max;
431
432     l2_errors = [];
433
434     % trapezoidal method
435     trapezoidal_method = IntegrationMethod();
436     trapezoidal_method.type = IntegrationType.Trapezoidal;
437     trapezoidal_method.gauss_points = 0; % not used for trapezoidal
438
439     trapezoidal_solution = NumericSolver.SolveNumeric(...
440         mesh, tmax, dt, theta, lhs_boundary, rhs_boundary, @(~, ~) 0.0,
441         trapezoidal_method);
442
443     % gaussian quadrature method
444     gaussian_method = IntegrationMethod();
445     gaussian_method.type = IntegrationType.Gaussian;
446     gaussian_method.gauss_points = 3; % 3-point Gaussian quadrature

```

```

447         gaussian_solution = NumericSolver.SolveNumeric(...
448             mesh, tmax, dt, theta, lhs_boundary, rhs_boundary, @(~, ~) 0.0,
            gaussian_method);
449
450         % compute L2 error
451         l2_error_trapezoidal = L2Error(analytical_solution, trapezoidal_solution);
452         l2_error_gaussian = L2Error(analytical_solution, gaussian_solution);
453         l2_errors = [l2_error_trapezoidal, l2_error_gaussian];
454
455         method_names = {"2-point Trapezoidal Integration", "3-point Gaussian
            Quadrature"};
456
457         Plotter.PlotL2Errors(l2_errors, "Gaussian vs Trapezoidal Integration", ...
458             "cw2/report/resources/part2/L2ErrorGaussianTrapezoidal", ...
459             method_names);
460     end
461
462     function Part2QuadraticBasisFunctions()
463         %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
464         %
465         % Function:      Part2TimeIntegrationComparison()
466         %
467         % Arguments:     None
468         % Returns:       None
469         %
470         % Description:   Runs a study comparing different time integration
471         %                 methods for Part 2 of the coursework.
472         %
473         %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
474
475
476
477     end
478
479 end
480
481 end
482

```

11. Mesh

11.1. Mesh.m

```

1 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
2 %
3 % ME40064 Coursework 2
4 %
5 % File      : Mesh.m
6 % Author    : samh25
7 % Created   : 2025-11-26 (YYYY-MM-DD)
8 % License   : MIT
9 % Description : A class defining a one-dimensional mesh for
10 %              finite element analysis.
11 %
12 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
13
14
15 classdef Mesh < handle
16     % inherit from handle to allow pass-by-reference
17
18     properties
19
20         xmin double
21         xmax double
22         dx double
23
24         order double
25
26         D double % diffusion coefficient
27         lambda double % reaction coefficient
28
29         node_count uint64
30         node_coords double % coordinates of global nodes
31
32         element_count uint64
33         elements MeshElement % array of mesh elements
34
35     end
36
37     methods
38
39         %% Mesh constructor
40         function obj = Mesh(xmin, xmax, element_count, order, D, lambda)
41
42             obj.xmin = xmin;
43             obj.xmax = xmax;
44             obj.dx = (xmax - xmin) / element_count;
45             obj.D = D;
46             obj.lambda = lambda;
47
48             obj.order = order;
49
50             % total number of nodes
51             obj.node_count = (element_count * order) + 1;
52             obj.node_coords = zeros(1, obj.node_count);
53
54             obj.element_count = element_count;
55             obj.elements = MeshElement.empty(element_count, 0);
56
57         end
58
59         function obj = Generate(obj)
60
61             disp('Generating normal mesh...');
62
63             % generate uniform node coordinates

```



```

64         obj.node_coords = linspace(obj.xmin, obj.xmax, obj.node_count);
65
66         % generate elements
67         for e = 1:obj.element_count
68
69             % determine global node IDs for this element
70             node_start = (e - 1) * obj.order + 1;
71             node_ids = node_start:(node_start + obj.order);
72
73             % coordinates for this element
74             coords = obj.node_coords(node_ids);
75
76             % create MeshElement object
77             obj.elements(e) = MeshElement(node_ids, coords, obj.order, obj.D,
obj.lambda);
78         end
79     end
80
81 end
82 end
83

```

11.2. MeshElement.m

```

1  %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
2  %
3  % ME40064 Coursework 2
4  %
5  % File      : MeshElement.m
6  % Author    : samh25
7  % Created   : 2025-11-26 (YYYY-MM-DD)
8  % License   : MIT
9  % Description : A class defining a one-dimensional mesh element
10 %
11 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
12
13 classdef MeshElement
14
15     properties
16
17         order      uint8    % polynomial order (1 = linear, 2 = quadratic)
18         node_ids    uint64   % global node IDs
19         node_coords double   % node coordinates
20         jacobian    double   % element jacobian d(x)/d(xi)
21         D           double   % diffusion coefficient
22         lambda      double   % reaction coefficient
23     end
24
25     methods
26
27         %% MeshElement constructor
28         function obj = MeshElement(ids, coords, order, D, lambda)
29
30             % assign properties
31             obj.node_ids = ids;
32             obj.node_coords = coords;
33             obj.order = order;
34             obj.D = D;
35             obj.lambda = lambda;
36
37             % linear mapping from [-1, 1] to [x1, x2]
38             % jacobian = dx/dxi = (x2 - x1) / 2
39             obj.jacobian = (coords(end) - coords(1)) / 2;
40
41         end

```

```

42     end
43 end
44
45

```

11.3. MultilayerMesh.m

```

1  %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
2  %
3  % ME40064 Coursework 2
4  %
5  % File      : Mesh.m
6  % Author    : samh25
7  % Created   : 2025-11-26 (YYYY-MM-DD)
8  % License   : MIT
9  % Description : A class defining a one-dimensional mesh for
10 %               finite element analysis.
11 %
12 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
13
14
15 classdef MultilayerMesh < Mesh
16     % inherit from handle to allow pass-by-reference
17
18     properties
19         layer_properties LayerProperties % array of layer properties
20     end
21
22     methods
23
24         %% Mesh constructor
25         function obj = MultilayerMesh(xmin, xmax, element_count, order, D, lambda,
layer_properties)
26
27             obj = obj@Mesh(xmin, xmax, element_count, order, D, lambda);
28             obj.layer_properties = layer_properties;
29
30         end
31
32         function obj = Generate(obj)
33
34             disp('Generating multilayer mesh...');
35
36             % generate uniform node coordinates
37             obj.node_coords = linspace(obj.xmin, obj.xmax, obj.node_count);
38
39             % generate elements
40             for e = 1:obj.element_count
41
42                 % determine global node IDs for this element
43                 node_start = (e - 1) * obj.order + 1;
44                 node_ids = node_start:(node_start + obj.order);
45
46                 % coordinates for this element
47                 coords = obj.node_coords(node_ids);
48
49                 midpoint = (coords(1) + coords(end)) / 2;
50
51                 % determine which layer this element is in
52                 layer_index = 1;
53
54                 for l = 1:length(obj.layer_properties)
55                     if midpoint >= obj.layer_properties(l).x
56                         layer_index = l;
57                     end

```

```

58         end
59
60         D = obj.layer_properties(layer_index).D;
61         lambda = -(obj.layer_properties(layer_index).beta +
obj.layer_properties(layer_index).gamma);
62
63         % create MeshElement object
64         obj.elements(e) = MeshElement(node_ids, coords, obj.order, D, lambda);
65     end
66 end
67
68 end
69 end
70
71

```

11.4. LayerProperties.m

```

1 classdef LayerProperties
2     properties
3         x      double % min x coordinate for this layer
4         D      double % diffusion coefficient
5         beta   double % extra-vascular diffusivity
6         gamma  double % drug degradation rate
7     end
8
9     methods
10        function obj = LayerProperties(x, D, beta, gamma)
11            obj.x = x;
12            obj.D = D;
13            obj.beta = beta;
14            obj.gamma = gamma;
15        end
16    end
17 end

```

12. Analytical

12.1. AnalyticalSolver.m

```

1 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
2 %
3 % ME40064 Coursework 2
4 %
5 % File      : AnalyticalSolver.m
6 % Author    : samh25
7 % Created   : 2025-11-26 (YYYY-MM-DD)
8 % License   : MIT
9 % Description : A static class defining an analytical solver
10 %             for the transient diffusion equation
11 %
12 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
13
14 classdef AnalyticalSolver
15
16     methods (Static)
17
18         function solution = SolveAnalytical(mesh, tmax, dt)
19
20             % time vector
21             time_vector = 0:dt:tmax;
22             solution = Solution(mesh, time_vector);
23
24             % loop over time steps
25             for step = 1:length(time_vector)
26
27                 t = time_vector(step);
28                 timestep_results = zeros(1, mesh.node_count);
29
30                 % loop over nodes
31                 for i = 1:mesh.node_count
32                     x = mesh.node_coords(i);
33                     timestep_results(i) = TransientAnalyticSoln(x, t);
34                 end
35
36                 solution.SetValues(timestep_results, step);
37             end
38         end
39     end
40 end
41 end

```

12.2. TransientAnalyticSoln.m

```

1 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
2 %
3 % ME40064 Coursework 2
4 %
5 % File      : TransientAnalyticSoln.m
6 % Author    : A. N. Cookson
7 % Created   : 2025-11-11 (YYYY-MM-DD)
8 % License   : -
9 % Description : Analytical solution to transient diffusion equation
10 %
11 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
12
13 function [ c ] = TransientAnalyticSoln(x,t)
14 %TransientAnalyticSoln Analytical solution to transient diffusion equation
15 % Computes the analytical solution to the transient diffusion equation for
16 % the domain x=[0,1], subject to initial condition: c(x,0) = 0, and Dirichlet
17 % boundary conditions: c(0,t) = 0, and c(1,t) = 1.
18 % Input Arguments:

```

```
19 % x is the point in space to evaluate the solution at
20 % t is the point in time to evaluate the solution at
21 % Output Argument:
22 % c is the value of concentration at point x and time t, i.e. c(x,t)
23
24 trans = 0.0;
25
26 for k=1:1000
27     trans = trans + (((-1)^k)/k) * exp(-k^2*pi^2*t)*sin(k*pi*x);
28 end
29
30 c = x + (2/pi)*trans;
31
32 end
```

13. Plotter

13.1. Plotter.m

```

1  %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
2  %
3  % ME40064 Coursework 2
4  %
5  % File      : Plotter.m
6  % Author    : samh25
7  % Created   : 2025-11-26 (YYYY-MM-DD)
8  % License   : MIT
9  % Description : A collection of static methods for plotting
10 %              results for the coursework.
11 %
12 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
13
14 classdef Plotter
15
16     methods (Static)
17
18         %% Plot entire solution as a heatmap - time as x-axis, position as y-axis and
19         %% solution value as color
20         function PlotHeatMap(solution, title_str, name, c_max)
21
22             set(0, "DefaultAxesFontSize", 12);
23             set(0, "DefaultTextFontSize", 12);
24
25             % Plot a heat map of the solution values over time
26             figure;
27             imagesc(solution.time, solution.mesh.node_coords, solution.values);
28             colorbar;
29             xlabel("Time (t)");
30             ylabel("Displacement (x)");
31             caxis([0 c_max]) % lock color axis for consistency
32             axis xy; % ensure y-axis is oriented correctly
33             title(title_str);
34             grid off;
35
36             set(gcf, 'Position', [0, 0, 500, 350]);
37
38             % Save figure
39             saveas(gcf, name, "png");
40             saveas(gcf, name, "fig");
41             openfig(name + ".fig");
42
43         end
44
45         %% Plot full solution at specified time samples
46         function PlotTimeSamples(solution, dt, time_samples, title_str, name)
47
48             set(0, "DefaultAxesFontSize", 12);
49             set(0, "DefaultTextFontSize", 12);
50
51             figure;
52             plot_handle = 0;
53
54             for i = 1:length(time_samples)
55                 t_sample = time_samples(i);
56
57                 step_index = round(t_sample / dt) + 1; % +1 for MATLAB indexing
58
59                 plot_handle = plot(solution.mesh.node_coords, solution.values(:,
60                                     step_index));
61                 set(plot_handle, "LineWidth", 1.5);
62
63                 hold on;

```

```

62         end
63
64         xlabel("Position (x)");
65         ylabel("c(x, t)");
66         title(title_str);
67
68         grid on;
69
70         legend_strings = cell(1, length(time_samples));
71         for i = 1:length(time_samples)
72             legend_strings{i} = ['t = ', num2str(time_samples(i))];
73         end
74
75         legend(legend_strings, "Location", "northwest");
76
77         set(gcf, 'Position', [0, 0, 500, 350]);
78
79         % Save figure
80         saveas(gcf, name, "png");
81         saveas(gcf, name, "fig");
82         openfig(name + ".fig");
83
84     end
85
86     %% Plot two solutions at a specific position over time
87     function PlotSampleOverTime(solution_1, solution_2, x_sample, title_str, name,
88     legend_strings)
89
90         set(0, "DefaultAxesFontSize", 12);
91         set(0, "DefaultTextFontSize", 12);
92
93         % find x index
94         x_index = round((x_sample - solution_1.mesh.xmin) / (solution_1.mesh.xmax -
95     solution_1.mesh.xmin) * solution_1.mesh.element_count) + 1; % +1 for MATLAB indexing
96
97         figure;
98         plot_handle = plot(solution_1.time, solution_1.values(x_index, :));
99         set(plot_handle, "LineWidth", 1.5);
100
101         hold on;
102
103         plot_handle = plot(solution_2.time, solution_2.values(x_index, :));
104         set(plot_handle, "LineWidth", 1.5);
105
106         xlabel("Time (t)");
107
108         ylabel("c(" + num2str(x_sample) + ", t)");
109         title(title_str);
110
111         grid on;
112
113         legend(legend_strings, "Location", "southeast");
114         set(gcf, 'Position', [0, 0, 500, 350]);
115
116         % Save figure
117         saveas(gcf, name, "png");
118         saveas(gcf, name, "fig");
119         openfig(name + ".fig");
120
121     end
122
123     function PlotConvergenceError(x_values, y_values, title_str, name, x_label,
124     y_label)
125
126         set(0, "DefaultAxesFontSize", 12);
127         set(0, "DefaultTextFontSize", 12);
128
129         figure;

```



```
126
127     plot_handle = loglog(x_values, y_values);
128     set(plot_handle, "LineWidth", 1.5);
129
130     xlabel(x_label);
131     ylabel(y_label);
132     title(title_str);
133     grid on;
134
135     set(gcf, 'Position', [0, 0, 500, 350]);
136
137     % Save figure
138     saveas(gcf, name, "png");
139     saveas(gcf, name, "fig");
140     openfig(name + ".fig");
141
142 end
143
144 function PlotL2Errors(l2_errors, title_str, name, legend_strings)
145
146     set(0, "DefaultAxesFontSize", 12);
147     set(0, "DefaultTextFontSize", 12);
148
149     figure;
150
151     for i = 1:length(l2_errors)
152         l2_error = l2_errors(i);
153         plot_handle = plot(l2_error.time, l2_error.l2_error);
154         set(plot_handle, "LineWidth", 1.5);
155         hold on;
156     end
157
158     xlabel("Time (t)");
159     ylabel("L2 Error");
160     title(title_str);
161
162     grid on;
163
164     legend(legend_strings, "Location", "northeast");
165     set(gcf, 'Position', [0, 0, 500, 350]);
166
167     % Save figure
168     saveas(gcf, name, "png");
169     saveas(gcf, name, "fig");
170
171     openfig(name + ".fig");
172
173 end
174
175 function PlotTwoConvergenceLines(x_values, y1_values, y2_values, title_str, name,
x_label, y_label, legend_strings)
176     set(0, "DefaultAxesFontSize", 12);
177     set(0, "DefaultTextFontSize", 12);
178
179     figure;
180
181     loglog(x_values, y1_values, '-o', 'LineWidth', 1.5, 'MarkerSize', 8);
182     hold on;
183     loglog(x_values, y2_values, '-s', 'LineWidth', 1.5, 'MarkerSize', 8);
184
185     xlabel(x_label);
186     ylabel(y_label);
187     title(title_str);
188     legend(legend_strings, 'Location', 'best');
189     grid on;
190
191     set(gcf, 'Position', [0, 0, 500, 350]);
```

```
192
193     saveas(gcf, name, "png");
194     saveas(gcf, name, "fig");
195     openfig(name + ".fig");
196     end
197
198     end
199 end
```

[illegible]


```
13
14 classdef DoseEvaluator
15
16     methods (Static)
17
18         function K = EvaluateSolution(solution, target_x, c_threshold, dt)
19
20             % first, find the closest node to the target
21             node_index = 0;
22
23             for i = 1:solution.mesh.node_count
24                 x = solution.mesh.node_coords(i);
25                 if x >= target_x
26                     node_index = i;
27                     break;
28                 end
29             end
30
31             fprintf("node index %d\n", node_index);
32             c = solution.values(node_index, :);
33
34             effective_t_index = 0;
35
36             for i = 1:length(c)
37                 if c(i) > c_threshold
38                     effective_t_index = i;
39                     break
40                 end
41             end
42
43             fprintf("effective t index %d\n", effective_t_index);
44
45             if effective_t_index == 0
46                 K = 0; % never exceeds threshold
47                 return;
48             end
49
50             % integrate concentration over time until effective_t_index
51             time_range = effective_t_index:length(solution.time);
52             K = trapz(c(time_range)) * dt;
53         end
54     end
55 end
```

15. Solver

15.1. NumericSolver.m

```

1 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
2 %
3 % ME40064 Coursework 2
4 %
5 % File      : NumericSolver.m
6 % Author    : samh25
7 % Created   : 2025-11-24 (YYYY-MM-DD)
8 % License   : MIT
9 % Description : Class definition for generic solver for the
10 %              transient diffusion-reaction equation
11 %
12 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
13
14
15 classdef NumericSolver
16
17     methods (Static)
18
19         function solution = SolveNumeric(mesh, tmax, dt, theta, left_boundary,
20             right_boundary, source_fn, integration_method)
21
22             % time vector
23             time_vector = 0:dt:tmax;
24             solution = Solution(mesh, time_vector);
25
26             % === SET INITIAL CONDITION EXPLICITLY ===
27             c0 = zeros(mesh.node_count, 1);
28             solution.SetValues(c0, 1); % column 1 = t=0
29
30             [K, M] = NumericSolver.CreateGlobalMatrices(mesh, theta, integration_method);
31
32             % loop over time steps
33             for step = 1:length(time_vector) - 1
34
35                 c_next = NumericSolver.SolveStep(mesh, solution, step, dt, theta, K, M,
36                     left_boundary, right_boundary, source_fn, integration_method);
37                 solution.SetValues(c_next, step + 1);
38
39             end
40
41         end
42
43         function c = SolveStep(mesh, solution, step, dt, theta, K, M, left_boundary,
44             right_boundary, source_fn, integration_method)
45
46             c_current = solution.values(:, step);
47
48             t = (step - 1) * dt; % current time, converted to 0-based index
49
50             % assemble system matrix and rhs vector
51             system_matrix = M + theta * dt * K;
52             rhs_vector = (M - (1 - theta) * dt * K) * c_current;
53
54             % add source term
55             f_current = NumericSolver.CreateSourceVector(mesh, t, source_fn,
56                 integration_method);
57             f_next = NumericSolver.CreateSourceVector(mesh, t + dt, source_fn,
58                 integration_method);
59             rhs_vector = rhs_vector + dt * (theta * f_next + (1 - theta) * f_current);
60
61             % apply boundary conditions

```

```

57     [system_matrix, rhs_vector] =
NumericSolver.ApplyBoundaryConditions(system_matrix, rhs_vector, t + dt, left_boundary,
right_boundary);
58
59     % solve system
60     c = system_matrix \ rhs_vector;
61
62     end
63
64     %% Create global stiffness and mass matrices
65     function [K, M] = CreateGlobalMatrices(mesh, theta, integration_method)
66
67         num_elements = mesh.element_count;
68         num_nodes = mesh.node_count;
69
70         % initialise global matrix (use sparse for efficiency with large systems)
71         K = sparse(num_nodes, num_nodes);
72         M = sparse(num_nodes, num_nodes);
73
74         for element_id = 1:num_elements
75
76             element = mesh.elements(element_id);
77             nodes = element.node_ids;
78             local_size = length(nodes);
79
80             diff_matrix = ElementMatrices.DiffusionElemMatrix(element,
integration_method);
81             react_matrix = ElementMatrices.ReactionElemMatrix(element,
integration_method);
82
83             k_matrix = diff_matrix - react_matrix;
84
85             elem_size = element.node_coords(end) - element.node_coords(1);
86             m_matrix = ElementMatrices.MassElemMatrix(element, integration_method);
87
88             % assemble into global matrices
89             for i = 1:local_size
90                 for j = 1:local_size
91                     gi = nodes(i); gj = nodes(j);
92                     K(gi, gj) = K(gi, gj) + k_matrix(i, j);
93                     M(gi, gj) = M(gi, gj) + m_matrix(i, j);
94                 end
95             end
96
97         end
98
99     end
100
101     %% Create source vector for given time
102     function F = CreateSourceVector(mesh, t, source_fn, integration_method)
103
104         F = zeros(mesh.node_count, 1);
105
106         % return if no source function defined
107         if (isempty(source_fn))
108             return;
109         end
110
111         for element_id = 1:mesh.element_count
112
113             element = mesh.elements(element_id);
114
115             elem_size = element.node_coords(end) - element.node_coords(1);
116             midpoint = (element.node_coords(1) + element.node_coords(end)) / 2;
117
118             f_val = source_fn(midpoint, t);
119

```



```

120         % Local Force Vector for linear element (Int N^T * s dx)
121         f_local = f_val * ElementMatrices.ForceMatrix(element, integration_method);
122
123         nodes = element.node_ids;
124         F(nodes) = F(nodes) + f_local;
125     end
126
127 end
128
129 function [lhs, rhs] = ApplyBoundaryConditions(lhs, rhs, t, left_boundary,
right_boundary)
130
131     % Store diagonal values before modification
132     diag_left = lhs(1,1);
133     diag_right = lhs(end,end);
134
135     % apply left boundary condition
136     switch left_boundary.Type
137
138     case BoundaryType.Dirichlet
139         lhs(1, :) = 0; % clear row
140         lhs(1, 1) = diag_left; % keep diagonal
141         rhs(1) = left_boundary.Value * diag_left; % scale by diagonal
142
143     case BoundaryType.Neumann
144         rhs(1) = rhs(1) + left_boundary.ValueFunction(t); % apply flux
145
146     end
147
148
149
150     % apply right boundary condition
151     switch right_boundary.Type
152     case BoundaryType.Dirichlet
153         lhs(end, :) = 0; % clear row
154         lhs(end, end) = diag_right; % set diagonal to 1
155         rhs(end) = right_boundary.Value * diag_right; % set value
156
157     case BoundaryType.Neumann
158         rhs(end) = rhs(end) + right_boundary.ValueFunction(t); % apply flux
159
160     end
161
162 end
163
164 end
165

```

15.2. BoundaryCondition.m

```

1 classdef BoundaryCondition
2     properties
3         Type BoundaryType % Boundary condition type (Dirichlet or Neumann)
4         Value double % Boundary condition value for Dirichlet
5         ValueFunction function_handle % Boundary condition function for Neumann - parameter
        t, return double
6     end
7 end

```

15.3. BoundaryType.m

```

1 classdef BoundaryType
2     enumeration
3         Dirichlet, Neumann

```

```

4   end
5 end

```

15.4. ElementMatrices.m

```

1 classdef ElementMatrices
2
3     methods (Static)
4
5         function matrix = DiffusionElemMatrix(element, method)
6
7             elem_size = element.node_coords(end) - element.node_coords(1);
8
9             if method.type == IntegrationType.Trapezoidal
10
11                 % create base matrix
12                 matrix = eye(element.order + 1);
13
14                 for i = 1:(element.order + 1)
15                     for j = 1:(element.order + 1)
16                         if i ~= j
17                             matrix(i, j) = -1;
18                         end
19                     end
20                 end
21
22                 % apply matrix scaling
23                 matrix = matrix * (element.D / elem_size);
24
25             else
26
27                 matrix = zeros(element.order + 1);
28                 [xi, wi] = ElementMatrices.GaussQuadraturePoints(method.gauss_points);
29
30                 for i = 1:length(xi)
31                     dN_dxi = ElementMatrices.ShapeFunctionDerivatives(element.order,
32                                     xi(i));
33
34                     J = element.jacobian;
35                     dN_dx = dN_dxi / J;
36
37                     % compute contribution to stiffness matrix
38                     matrix = matrix + (element.D * (dN_dx' * dN_dx)) * (wi(i) * J);
39                 end
40             end
41         end
42     end
43
44     function matrix = ReactionElemMatrix(element, method)
45
46         elem_size = element.node_coords(end) - element.node_coords(1);
47
48         if method.type == IntegrationType.Trapezoidal
49
50             % create base matrix
51             matrix = eye(element.order + 1) * 2;
52
53             for i = 1:(element.order + 1)
54                 for j = 1:(element.order + 1)
55                     if i ~= j
56                         matrix(i, j) = 1;
57                     end
58                 end
59             end

```

```

60
61     % apply matrix scaling
62     matrix = matrix * (element.lambda * elem_size / 6);
63
64     else
65
66         matrix = zeros(element.order + 1);
67         [xi, wi] = ElementMatrices.GaussQuadraturePoints(method.gauss_points);
68
69         for i = 1:length(xi)
70             N = ElementMatrices.ShapeFunctions(element.order, xi(i));
71
72             J = element.jacobian;
73
74             % compute contribution to stiffness matrix
75             matrix = matrix + (element.lambda * (N' * N)) * (wi(i) * J);
76         end
77     end
78 end
79
80 function matrix = MassElemMatrix(element, method)
81
82     elem_size = element.node_coords(end) - element.node_coords(1);
83
84     if method.type == IntegrationType.Trapezoidal
85
86         % create base matrix
87         matrix = eye(element.order + 1) * 2;
88
89         for i = 1:(element.order + 1)
90             for j = 1:(element.order + 1)
91                 if i ~= j
92                     matrix(i, j) = 1;
93                 end
94             end
95         end
96
97         % apply matrix scaling
98         matrix = matrix * (elem_size / 6);
99
100    else
101
102        matrix = zeros(element.order + 1);
103        [xi, wi] = ElementMatrices.GaussQuadraturePoints(method.gauss_points);
104
105        for i = 1:length(xi)
106            N = ElementMatrices.ShapeFunctions(element.order, xi(i));
107
108            J = element.jacobian;
109
110            % compute contribution to stiffness matrix
111            matrix = matrix + (N' * N) * (wi(i) * J);
112        end
113
114    end
115
116 end
117
118 function matrix = ForceMatrix(element, method)
119
120     elem_size = element.node_coords(end) - element.node_coords(1);
121
122     if method.type == IntegrationType.Trapezoidal
123
124         % create base matrix
125         matrix = ones(element.order + 1, 1);
126

```

```

127         % apply matrix scaling
128         matrix = matrix * (elem_size / 2);
129
130     else
131
132         matrix = zeros(element.order + 1, 1);
133         [xi, wi] = ElementMatrices.GaussQuadraturePoints(method.gauss_points);
134
135         for i = 1:length(xi)
136             N = ElementMatrices.ShapeFunctions(element.order, xi(i));
137
138             J = element.jacobian;
139
140             % compute contribution to stiffness matrix
141             matrix = matrix + N' * (wi(i) * J);
142         end
143     end
144 end
145
146 end
147
148
149 methods (Static, Access = private)
150
151     function [xi, wi] = GaussQuadraturePoints(n)
152
153         switch n
154             case 1
155                 xi = 0;
156                 wi = 2;
157             case 2
158                 xi = [-1/sqrt(3), 1/sqrt(3)];
159                 wi = [1, 1];
160             case 3
161                 xi = [-sqrt(3/5), 0, sqrt(3/5)];
162                 wi = [5/9, 8/9, 5/9];
163             otherwise
164                 error('Gauss quadrature for n > 3 not implemented.');

```

```
194     end
195 end
```

15.5. IntegrationMethod.m

```
1 classdef IntegrationMethod
2     properties
3         type          IntegrationType
4         gauss_points  uint8
5     end
6 end
```

15.6. IntegrationType.m

```
1 classdef IntegrationType
2     enumeration
3         Trapezoidal, Gaussian
4     end
5 end
```

16. Tests

16.1. NumericSolverTest.m

```

1 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
2 %
3 % ME40064 Coursework 2
4 %
5 % File      : NumericSolverTest.m
6 % Author    : samh25
7 % Created   : 2025-11-27 (YYYY-MM-DD)
8 % License   : MIT
9 % Description : Test suite for NumericSolver class
10 %
11 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
12
13 function tests = NumericSolverTest
14     tests = functiontests(localfunctions);
15 end
16
17 function TestSolveNumericReactionOnly(testCase)
18
19     % mesh parameters
20     xmin = 0.0;
21     xmax = 1.0;
22     element_count = 6;
23     order = 1;
24     lambda = -1.0;
25     D = 0.0;
26
27     % time parameters
28     tmax = 0.5;
29     dt = 0.02;
30     theta = 0.5; % Crank-Nicholson
31
32     % generate mesh
33     mesh = Mesh(xmin, xmax, element_count, order, D, lambda);
34     mesh.Generate();
35
36     % solver parameters
37     lhs_boundary = BoundaryCondition();
38     lhs_boundary.Type = BoundaryType.Neumann;
39     lhs_boundary.ValueFunction = @(t) 0.0;
40
41     rhs_boundary = BoundaryCondition();
42     rhs_boundary.Type = BoundaryType.Neumann;
43     rhs_boundary.ValueFunction = @(t) 0.0;
44
45     integration_method = IntegrationMethod();
46     integration_method.type = IntegrationType.Trapezoidal;
47     integration_method.gauss_points = 0; % not used for trapezoidal
48
49     numeric_solution = NumericSolver.SolveNumeric(...
50         mesh, tmax, dt, theta, lhs_boundary, rhs_boundary, @SourceFunction,
51         integration_method);
52
53     % analytical solution
54     t_analytic = 0:dt:tmax;
55     c_exact = 10 * (1 - exp(lambda * t_analytic));
56
57     % chose random node (3 in this case) to compare
58     c_numeric = numeric_solution.values(3,:);
59     error = norm(c_numeric - c_exact) / norm(c_exact);
60
61     tolerance = 1e-3;
62     verifyLessThan(testCase, error, tolerance);
63 end

```

```
63  
64 function s = SourceFunction(x, t)  
65     s = 10;  
66 end  
67
```