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Comparison of Semi-Implicit and Fully-Implicit 2 Methods for Solving PDE-ODE Coupled Systems

3 by

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²⁸ **Chapter 1**

²⁹ **Model Definition**

³⁰ **1.1 History**

³¹ The tradition biofilm model has been continually developed over many iterations since 1980. Rittmann
³² and McCarty (1980) formulated the steady-state biofilm model, developed using the concept that
³³ biofilm growth would be the result of a steady flux from substrate. Since then the model have evolved
³⁴ to include modelling three-dimensional growth of multispecies anaerobic biofilms (Noguera et al.
³⁵ (1999)) and spatially heterogeneous biofilm structures (Eberl et al. (2001)).

³⁶ The modelling of *Clostridium Thermocellum* is unique because this cellulolytic anaerobic bacteria
³⁷ does not generate an extracellular polymeric substance. This uncharacteristic behaviour means that
³⁸ the mathematical model based on the work of Eberl and Demaret (2007) cannot be used as is. They
³⁹ modelled the biomass density and nutrient concentrations as a two-PDE-coupled system. Recently,
⁴⁰ Wang et al. (2011), used a cellular automata based model for simulating the growth of *Clostridium*
⁴¹ *Thermocellum*. From this, better results were thought to derive from a continuous differential equa-
⁴² tion based model. Here the spatial diffusion of the substrait concentration is removed to mimic the
⁴³ carbon substrait that is consumed by *Clostridium Thermocellum*. This results in a PDE-ODE-coupled
⁴⁴ system. This is based on the work done by Dumitrache (2014), where this same coupling was used
⁴⁵ and formulated.

⁴⁶ 1.2 Model Description

⁴⁷ The model used for simulations is based on the deterministic model developed in Eberl et al. (2001),
⁴⁸ which was designed to simulate the development of spatially heterogeneous biofilm structures. They
⁴⁹ modelled the biomass density and nutrient concentration as a two-PDE-coupled system. Here the spa-
⁵⁰ tial diffusion of the nutrient concentration is removed to mimic the carbon substrate that *C.Thermocellum*
⁵¹ consumes in growth. This makes a PDE-ODE-coupled system purposed as,

$$M = \nabla_x (d(M) \nabla_x M) + f(C)M \quad (1.1)$$

$$C = -g(C)M \quad (1.2)$$

⁵² where

$$d(M) = d \frac{M^\alpha}{(1 - M)^\beta} \quad (1.3)$$

$$f(C) = u \frac{C}{k + C} - n \quad (1.4)$$

$$g(C) = y \frac{C}{k + C} \quad (1.5)$$

⁵⁸ Here we have a pair of equations, (1.1) and (1.2), that represent the biomass density and substrate
⁵⁹ concentration respectively. The spatial diffusion of the biofilm is modelled with density-dependent
⁶⁰ diffusion, represented by (1.3), and the growth rate of biomass is given by (1.4). The growth rate is
⁶¹ simple Monod kinetic growth with a constant death rate. In (1.2) there is only a consumption term
⁶² from the bacteria consuming the carbon substrate. This term is based on the growth of the biomass,
⁶³ differing only by a scalar multiplier.

⁶⁴ The dimensions of the parameters and variables are in Table 1.1.

Variable/Parameter	Dimensions
t	[days]
x	[meters]
M	[$\frac{\text{grams}}{\text{meters}^3}$]
C	[$\frac{\text{grams}}{\text{meters}^3}$]
d	[$\frac{\text{meters}^2}{\text{days}}$]
α	[$-$]
β	[$-$]
u	[days^{-1}]
k	[$\frac{\text{grams}}{\text{meters}^3}$]
y	[$\frac{C}{M}$]
n	[$\frac{\text{grams}}{\text{meters}^3 \cdot \text{days}}$]

Table 1.1: List of parameters and their dimensions

65 1.3 Nondimensionalization

66 To help facilitate the analyses of this system, the full removal of all physical units is preferred. This
 67 process of nondimensionalization involves using known parameters to create substitutions with phys-
 68 ical units cancelling. Here the parameters used are: the biomass growth rate, u ; the length of the
 69 region, L ; and the maximum density for biomass and substrait, M_∞ and C_∞ . From using the follow-
 70 ing parameter changes, the system can be made unitless.

$$\chi = \frac{x}{L} \implies L d\chi = dx \quad (1.6)$$

$$\tau = ut \implies \frac{1}{u} d\tau = dt \quad (1.7)$$

$$\mathcal{M} = \frac{M}{M_\infty} \quad (1.8)$$

$$\mathcal{C} = \frac{C}{C_\infty} \quad (1.9)$$

$$\delta = \frac{1}{uL^2} d \quad (1.10)$$

$$\kappa = \frac{k}{C_\infty} \quad (1.11)$$

$$\nu = \frac{n}{uC_\infty} \quad (1.12)$$

$$\gamma = \frac{M_\infty}{C_\infty} y \quad (1.13)$$

⁷¹ Using these, (1.1) and (1.2) can be simplified and nondimensionalized into,

$$\mathcal{M}_\tau = \nabla_\chi (D(\mathcal{M}) \nabla_\chi \mathcal{M}) + F(\mathcal{C}) \mathcal{M} \quad (1.14)$$

$$\mathcal{C}_\tau = -G(\mathcal{C}) \mathcal{M}, \quad (1.15)$$

⁷² where,

$$\begin{aligned} D(\mathcal{M}) &= \delta \frac{\mathcal{M}^\alpha}{(1 - \mathcal{M})^\beta} \\ F(\mathcal{C}) &= \frac{\mathcal{C}}{\kappa + \mathcal{C}} - \nu \\ G(\mathcal{C}) &= \gamma \frac{\mathcal{C}}{\kappa + \mathcal{C}}. \end{aligned} \quad (1.16)$$

⁷⁴ with only $\delta, \kappa, \nu, \gamma$ as model parameters.

75 1.4 Parameters

76 Each of the dimensionless parameters in (1.16) have a biological representation based on the transfor-
77 mations done. The parameter δ is the dimensionaless constant for diffusion. It affects the change in
78 biomass from adjacent biomass sources, a greater δ results in a greater change. The parameter κ is the
79 half-saturation point, it is exactly the value for which substrait concentration results in 0.5-optimum
80 growth rate. Parameter ν is the death rate of the biomass. Specifically, it is the ratio of biomass
81 growth to death, representing the fraction of biomass density that perishes from natural causes or a
82 lack of substrait. Lastly, γ is the yield ratio. It signifies the ratio of substrait consumed to biomass
83 growth. Here, a larger γ value results in more substrait being consumed to produce the same amount
84 of biomass.

85 With (1.14) being reduced to four parameters the numerical analysis become more simiplified while
86 still retaining the same significance in results.

87 **Chapter 2**

88 **Numerical Methods**

89 **2.1 Discretization**

90 In order to find the solution for (1.14) spatial and temporal discretizations must be made. First the
91 equations are discretized in time,

$$\frac{M^{k+1} - M^k}{\Delta t} = \nabla_x(D(M^{k+1})\nabla_x M^{k+1}) + F(C^{k+1})M^{k+1}, \quad (2.1)$$

$$\frac{C^{k+1} - C^k}{\Delta t} = \frac{h}{2}(G(C^{k+1})M^{k+1} + G(C^k)M^k). \quad (2.2)$$

95 Here, (2.1) follows the ideas of the Backwards Euler Method; (2.2) follows Trapezoidal Rule. The
96 index variable k has also been introduced in (2.1 - 2.2) such that $M^k(x) \approx M(t^k, x)$, allowing an
97 approximation at a certain time, t^k , to be used; this reduces the dimensionality of the problem.

98 For this system, the region of consideration will be a rectangular region, Ω . This region has Neumann
99 boundary conditions, $\frac{\partial M}{\partial x} = \frac{\partial C}{\partial x} = 0, \forall x \in \partial\Omega$. Now, only (2.1) requires spatial considerations
100 since, according to the biology of our system, the substrate does not diffuse across the region. The
101 spatial discretization will be through the Finite Difference Method as described in Saad (2003). Here,
102 a uniform $n \times m$ grid is used to discretize Ω . Since all the calculations will be done on the grid
103 intersections the discretization will be grid-point based. This means that a $n \times m$ grid implies there

104 are $(n - 1) \times (m - 1)$ grid boxes. The distance between grid points is the same in both x_1 and x_2
 105 dimensions; we have $\Delta x_1 = \Delta x_2$. A five-point stencil is used to approximate the solution of (2.1) at
 106 each grid point. To index the grid point, i and j are used such that $M_{i,j}^k \approx M(t^k, x_{1_i}, x_{2_j})$. To account
 107 for the dependency on neighbouring grid points, we introduce σ as the index pair from the set

$$108 \quad \mathcal{N}_{ij} = \{n_{ij}, e_{ij}, s_{ij}, w_{ij}\}. \quad (2.3)$$

109 where,

$$110 \quad n_{ij} = \begin{cases} (i, j + 1) & \text{if } j < m \\ (i, j - 1) & \text{if } j = m \end{cases} \quad e_{ij} = \begin{cases} (i + 1, j) & \text{if } i < n \\ (i - 1, j) & \text{if } i = n \end{cases} \quad (2.4)$$

$$s_{ij} = \begin{cases} (i, j - 1) & \text{if } j > 0 \\ (i, j + 1) & \text{if } j = 0 \end{cases} \quad w_{ij} = \begin{cases} (i - 1, j) & \text{if } i > 0 \\ (i + 1, j) & \text{if } i = 0 \end{cases}.$$

111 With \mathcal{N}_{ij} and σ we can account for the difference in boundary points and interior points.

112 The equation for (2.1), after spatial discretization, is

$$113 \quad \frac{M_{i,j}^{k+1} - M_{i,j}^k}{\Delta t} = \frac{1}{\Delta x^2} \sum_{\sigma \in \mathcal{N}_{ij}} \left(\frac{D(M_{\sigma}^{k+1}) + D(M_{i,j}^{k+1})}{2} \right) \cdot (M_{\sigma}^{k+1} - M_{i,j}^{k+1}) + F(C_{i,j}^{k+1}) M_{i,j}^{k+1} \quad (2.5)$$

114 For (2.5), the arithmetic mean of the diffusion function, D , is taken because of the steep gradiant at
 115 the interface. The alternative would be to use $D(M_{i+\frac{s}{2},j+\frac{r}{2}}^{k+1})$, however this may result in a value of
 116 zero and thus nullify the effect of the spatial diffusion.

117 2.2 Solving Method

118 Now there exist equations for which C and M can be solved, (2.2) and (2.5) respectivly. Using C^k and
 119 $M_{i,j}^k$ as approximations of the solutions for (1.14) will allow the system to be solved by computing
 120 C^{k+1} and $M_{i,j}^{k+1}$. However, there are complications with trying to get an explicit formula for $M_{i,j}^{k+1}$
 121 from (2.5) because of the dependency on M in $D(M)$. To remedy this, a fixed point iteration is

introduced. In a single time step, the solutions for M and C can be solved using the previous time step solution in the follow manner:

$$\frac{M_{i,j}^{(p+1)} - M_{i,j}^k}{\Delta t} = \frac{1}{\Delta x^2} \sum_{(s,r) \in \mathbb{A}} \left(\frac{D(M_{i+s,j+r}^{(p)}) + D(M_{i,j}^{(p)})}{2} \cdot (M_{i+s,j+r}^{(p+1)} - M_{i,j}^{(p+1)}) \right) + F(C_{i,j}^{(p)}) M_{i,j}^{(p+1)} \quad (2.6)$$

$$\frac{C^{(p+1)} - C^k}{\Delta t} = \frac{-1}{2} (G(C^{(p+1)}) M^{(p+1)} + G(C^k) M^k) \quad (2.7)$$

where $(p) \in (0, 1, \dots, P)$. Note, that the equation for $M_{i,j}^{(p+1)}$ shown in (2.6) refers to the interior points only. A similar change is done for the boundary points but is not shown due to its complexity. It is important to show explicitly that the purpose of the fixed point iteration is to link two distinct times with P solutions in between them, such that:

$$\begin{aligned} M^{(p=0)} &= M^k, & M^{(p=P)} &= M^{k+1}, \\ C^{(p=0)} &= C^k, & C^{(p=P)} &= C^{k+1}. \end{aligned} \quad (2.8)$$

In this fixed point format, given by (2.6 - 2.7), the equations can be rearrange and solved by conventional methods.

For (2.6), a linear system of equations can be created following Saad (2003). For each grid point (i, j) a linear system exists, defined as:

$$\begin{aligned} \frac{M_{i,j}^k}{\Delta t} &= \sum_{(i,j) \in \mathbb{A}} \left(\frac{D(M_{i+s,j+r}^{(p+1)}) + D(M_{i,j}^{(p+1)})}{2\Delta x^2} \cdot M_{i+s,j+r}^{(p+1)} \right) \\ &+ \left(\sum_{(i,j) \in \mathbb{A}} \left(\frac{D(M_{i+s,j+r}^{(p+1)}) + D(M_{i,j}^{(p+1)})}{2\Delta x^2} \right) - F(C_{i,j}^{(p)}) + \frac{1}{\Delta t} \right) M_{i,j}^{(p+1)}. \end{aligned} \quad (2.9)$$

¹³⁷ From (2.9), a five-diagonal matrix can be created defined as,

$$\text{138 } A = \begin{pmatrix} a_{i,j} & a_{i+1,j} & & a_{i,j+1} & & \\ a_{i-1,j} & \ddots & \ddots & & \ddots & \\ & \ddots & \ddots & \ddots & & \ddots \\ a_{i,j-1} & & a_{i-1,j} & a_{i,j} & a_{i+1,j} & a_{i,j+1} \\ & \ddots & & \ddots & \ddots & \ddots \\ & & a_{i,j-1} & a_{i-1,j} & a_{i,j} & a_{i+1,j} & a_{i,j+1} \\ & & & \ddots & \ddots & \ddots & \ddots \\ & & & & \ddots & \ddots & \ddots & a_{i+1,j} \\ & & & & a_{i,j-1} & a_{i-1,j} & a_{i,j} & \\ \end{pmatrix} \quad (2.10)$$

¹³⁹ where each $a_{i,j}$ is the coefficient based on (2.9).

¹⁴⁰ Solving (2.10) can be done by use of the Conjugate Gradient method provided that certain conditions
¹⁴¹ are satisfied.

¹⁴² **Proposition 2.2.1.** *The matrix A , (2.10), is positive definite and symmetric when $\frac{1}{F(C_{i,j}^{(p)})} < \Delta t$.*

¹⁴³ *Proof.* Matrix A is positive definite if all the eigenvalues are positive. Using the Circle theorem
¹⁴⁴ described by Geršgorin (1931), the eigenvalues can be shown to be positive if, independently on all
¹⁴⁵ rows, the sum of the off-diagonals values is less than the diagonal value. This can be verified. From
¹⁴⁶ (2.9) it can be said that,

$$\text{147 } \sum_{(i,j) \in \mathbb{A}} \left(\frac{D(M_{i+\frac{s}{2}, j+\frac{r}{2}}^{(p)})}{\Delta x^2} \right) < \left(\sum_{(i,j) \in \mathbb{A}} \left(\frac{D(M_{i+\frac{s}{2}, j+\frac{r}{2}}^{(p)})}{\Delta x^2} \right) - F(C_{i,j}^{(p)}) + \frac{1}{\Delta t} \right). \quad (2.11)$$

¹⁴⁸ This simplifies to,

$$\text{149 } F(C_{i,j}^{(p)}) < \frac{1}{\Delta t} \quad (2.12)$$

¹⁵⁰ The symmetry of A can be trivially shown if one considers the formation of the diagonals. On a

151 single row, each element corresponds to the adjacent grid points of grid i, j . As the grid ordering
 152 counts along, the elements that are equidistance from the diagonal are actually reference to the same
 153 grid point. Therefore we have symmetry. \square

154 It is important to remark that even though there is a condition for which matrix A is positive definite
 155 and symmetric, it realistically will never occur. The condition, $\frac{1}{F(C)} < \Delta t$, relates the growth of
 156 the biomass to the size of timestep selected. Specifically, if a large enough time step is choosen,
 157 then A is not guarenteed to converge. When this occurs, it means that a time step, larger then the
 158 characteristic growth rate of the biomass, has been incorrectly choosen. This means that the there
 159 would be no relavent results since all the growth, and subsequent reactions, would have occured in a
 160 single timestep.

161 Given that A is positive definite and symmetric, the conjugate gradiant method can be used to compute
 162 the solution. As an added property, A also happens to be diagonally dominate. This results in A being
 163 a M-matrix. It also means that it could be solved using Bi-Conjugate Gradient Method. However
 164 the Conjugate Gradient method has a faster computation time then Bi-Conjugate Gradiant method for
 165 this problem and is used for this reason (Barrett et al. (1987)).

166 For solving (2.7), the equation can be rearranged into a quadratic form, substituting in $G(C)$ from
 167 (1.16)

$$168 \quad (C^{(p+1)})^2 + \left(\kappa - C^k + \frac{h}{2} \gamma M^{(p+1)} + \frac{h \gamma C^k M^k}{2 \kappa + C^k} \right) C^{(p+1)} + \left(-\kappa C^k + \frac{h \gamma \kappa C^k M^k}{2 \kappa + C^k} \right) = 0. \quad (2.13)$$

169 Using the quadratic equation results in,

$$170 \quad C^{(p+1)} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \quad (2.14)$$

¹⁷¹ for which,

$$a = 1$$

$$\begin{aligned} \text{172} \quad b &= \kappa - C^k + \frac{h}{2} \gamma M^{(p+1)} + \frac{h}{2} \frac{\gamma C^k M^k}{\kappa + C^k} \\ c &= -\kappa C^k + \frac{h}{2} \frac{\gamma \kappa C^k M^k}{\kappa + C^k} \end{aligned} \quad (2.15)$$

¹⁷³ To determine which branch of (2.14) to use, a physical situation is used. Specifically the case where
¹⁷⁴ there exist no biomass, $M = 0$. The expected outcome is that no substrate is consumed and thus
¹⁷⁵ the substrait concentration will remain constant as a function of t . When the equations in (2.15) are
¹⁷⁶ evaluated at $M = 0$, the result it,

$$\text{177} \quad a = 1, \quad b = \kappa - C^k, \quad c = -\kappa C^k, \quad (2.16)$$

¹⁷⁸ which can be used to evaluate (2.14) as,

$$\begin{aligned} \text{179} \quad C^{(p+1)} &= \frac{-(\kappa - C^k) \pm \sqrt{(\kappa - C^k)^2 - 4(-\kappa C^k)}}{2} \\ &= \frac{1}{2} \left(C^k - \kappa \pm \sqrt{\kappa^2 + 2\kappa C^k + (C^k)^2} \right) \\ &= \frac{1}{2} (C^k - \kappa \pm (\kappa + C^k)). \end{aligned} \quad (2.17)$$

¹⁸⁰ Now, if the positive branch is used the above equation evaluates to $C^{(p+1)} = C^k$. This means that
¹⁸¹ between any two distinct times, the substrait concentration will remain constants, which was expected.
¹⁸² To further this confirmation, the negative branch results in $C^{(p+1)} = -\kappa$, a non-postive substrate
¹⁸³ concentration, which is not physically relavent.

$$\text{184} \quad C^{(p+1)} = \frac{-b + \sqrt{b^2 - 4ac}}{2a} \quad (2.18)$$

¹⁸⁵ where a, b , and c are defined in (2.15).

¹⁸⁶ Now that computable solutions for M and C at a single time step have been found, an algorithm to
¹⁸⁷ solve for the next time step can be established. Algorithm 1 shows the organization of solving (2.7 -

2.6).

Data: M^k, C^k are the values from the previous timestep and $p = 0$.

begin

```

Let  $M^{(0)} = M^k$  and  $C^{(0)} = C^k$ ;
while Convergence is not achieved do
    Solve  $A^{(p)}M^{(p+1)} = b^{(p)}$ ;
    Solve  $C^{(p+1)} = \frac{1}{2}(2b \pm \sqrt{b^2 - 4c})$ ;
    Check convergence;
    Let  $C^{(p)} = C_{(p+1)}$ ;
    Let  $M^{(p)} = M_{(p+1)}$ ;
    Let  $p = p + 1$ ;
end
Let  $M^{(k+1)} = M^{(P)}$  and  $C^{(k+1)} = C^{(P)}$ ;
end
```

Algorithm 1: Algorithm for the fully-implicit solving of (1.14)

188

189 Note that Algorithm 1 actually describes both a fully- and semi- implicit method for solving (1.14).

190 If $P = 1$ then only a single iteration of the algorithm is applied, which correlates to a semi-implicit
 191 method would behave. This would result in a change similar to how the Gauss-Seidal method changes
 192 the Jacobi method; the values used would no longer be updated in a single timestep when $P = 1$.

193 To use the algorithm, the matrix system was converted into a 1D array by use of a bijective mapping
 194 defined as:

$$\begin{aligned} \pi : \{0, \dots, n\} \times \{0, \dots, m\} &\rightarrow \{0, \dots, nm\} \\ 195 \quad (i, j) &\rightarrow \pi(i, j) \end{aligned} \tag{2.19}$$

196 This mapping allows the system to be easily stored in diagonal format, since (2.10) has five distinct
 197 diagonals.

198 2.3 Computational Setup

199 The implementation of Algorithm 1 was done with Fortran.

200 All the computations were run on a custom built workstation with an Intel Xeon CPU E5-2650 (1.2
 201 GHz, 20MB cache size) and 32 GB RAM under Red Hat Enterprise Linux Server release 6.5 (San-

202 tiago). Running the computations with OpenMP, took advantage of 6 out of the 16 processors of the
 203 Intel Xeon CPU, each with 2 threads. The GNU Fortran compiler, version 4.4.7, was used for all
 204 computations; the compiler arguments were

205 `-O3 -fdefault-real-8 -fopenmp`

206 2.4 Method Validation

207 With a defined method and computational setup a variety of simulations can be run to observe the
 208 accuracy and behaviour of the method. An examination of a typical simulation will show if the ex-
 209 pected behaviour is observed, validating the method as functioning. A convergence analysis for the
 210 method can be done to confirm that solutions from different grid sizes approach a single solution as
 211 they become more precise. This convergence test will also show the thresholds for an accurate simu-
 212 lation result, to help reduce the computation times. With a well-established method, the comparison
 213 between semi- and fully-implicit methods can be done.

214 2.4.1 Basic Simulations

215 Using Algorithm 1, simple scenarios can be tested as a first verification on the method.

216 A simple test would be to check if the spatial discretization can preserve specific characteristics of the
 217 solutions. One example of this would be seeing if a 1D initial condition could be preserved as time
 218 progresses. Having all of the biomass on one boundary of Ω , for example across the y -axis, would
 219 qualify as a 1D initial condition. These initial conditions will be defined as:

$$220 M = \begin{cases} -\left(\frac{h}{d^4}\right)x^4 + h & , \text{if } y \leq d \\ 0 & , \text{otherwise} \end{cases} \quad (2.20)$$

$$C = 1$$

221 where $h = 0.1$ and $d = \frac{5}{128}$. Here, h and d represent the height and depth of the inoculation site.

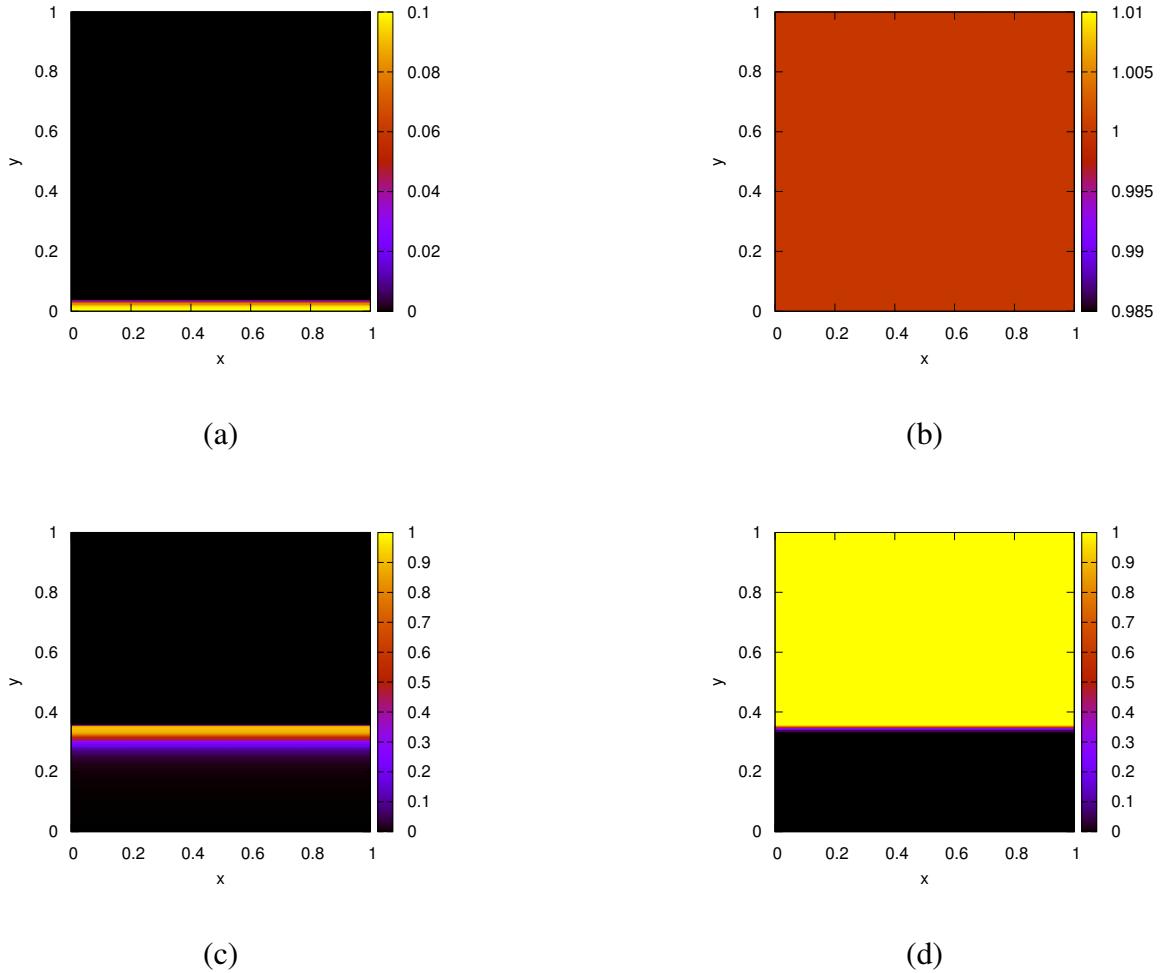


Figure 2.1: Solutions for (ac) M and (bd) C with 1D initial conditions defined in (2.20) at (ab) $t = 0$ and (cd) $t = 40$. Computed with a 1025×1025 grid and a timestep of $\Delta t = 10^{-3}$.

222 The solution shown in Figure 2.1 shows that the 1D characteristic of the biomass stays at a later time.
 223 Another characteristic to observe would be if a spherical initial condition remains spherical. Using
 224 intial conditions for the biomass,

$$225 \quad M = \begin{cases} -\frac{h}{d^2} (x - 0.5)^2 + (y - 0.5)^2 + h & , \text{if } (x - 0.5)^2 + (y - 0.5)^2 < d^2 \\ 0 & , \text{otherwise} \end{cases}, \quad (2.21)$$

226 a test can be tried to see if the spherical nature of the solution is kept as time progresses. This can be
 227 seen in Figure 2.2, where at different times the shape of the biomass, M , is seen to remain spherical.

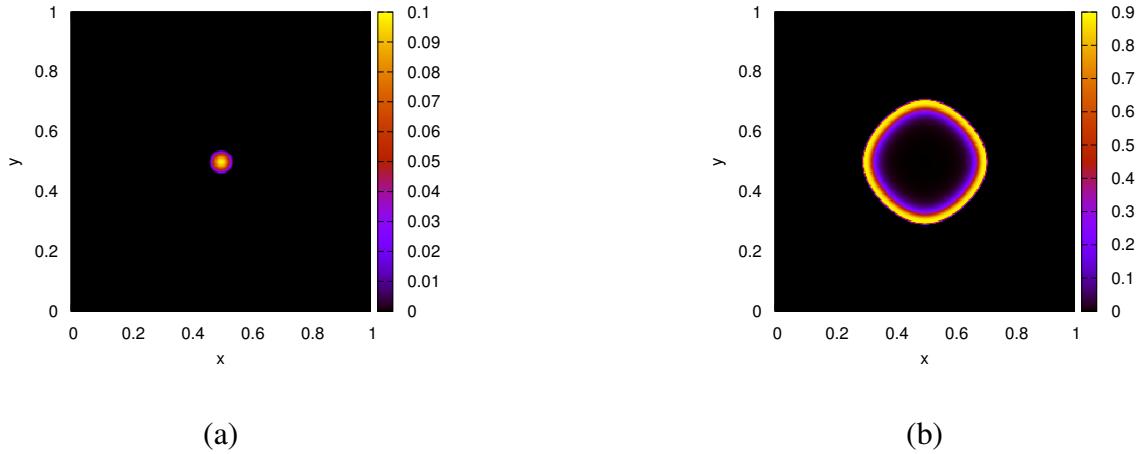


Figure 2.2: Solutions for M with spherical initial conditions defined by (2.21) at (a) $t = 0$ and (b) $t = 40$. Computed with a 1025×1025 grid and a timestep of $\Delta t = 10^{-3}$.

Both Figure 2.1 and Figure 2.2 increase the confidence that the spatial discretization did not introduce any loss of characteristics for the solutions.

Given the boundary conditions and spatial discretization, there could be a possible source or sink of biomass when it must diffuse along the boundary of the region. To ensure this is not the case, the total amount of biomass can be used to compare the simulated amount against the theoretical amount. However, the total biomass cannot be exactly determined with the given growth rate function. This means that there will not be anything to measure the validity of the simulation solution against. If we let the growth rate be some constant called a , the expected total biomass would be of the form $y_0 e^{at}$. This can be checked by tracking the total biomass, now called $T_M(t)$, with the changed growth rate function, $F(C) = a$. The calculation of $T_M(t)$ can be done by,

$$T_M(t) = \int_{\Omega} M(t) dx. \quad (2.22)$$

Numerically, this is computed by grid-wise summation,

$$T_M(t^k) \approx T_M^k = \frac{\sum_i^n \sum_j^m M_{i,j}^k}{nm}. \quad (2.23)$$

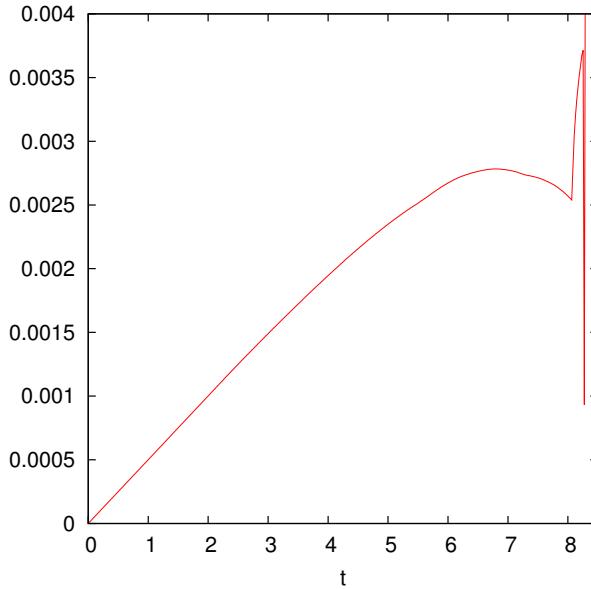


Figure 2.3: Plot of the relative error, $\frac{|f_1 - f_2|}{|f_2|}$, between the computed total biomass, $f_1 = T_M(t)$, and the theoretical total biomass, $f_2 = y_0 e^x$. The changes after $t = 8$ are from the biomass having completely filled the region Ω . This means that there is no physical space for the biomass to occupy and thus the growth slows down to a stop.

241 The simulation setup used will be analogous to that used for Figure 2.2. The one difference will be
 242 that the simulation here is ran for a longer time to allow the biomass to diffuse along the boundary,
 243 showing the boundary effects.

244 From Figure 2.3 we can see that the total biomass only differs between the computed value and the
 245 theoretical value by a relative error less than 0.003. The cases where the error becomes significant are
 246 from the region being completely filled with biomass, at which point diffusion is no longer possible.
 247 The error fluctuates violently here because of this. This suggests that the method does not introduce
 248 any significant sources or sinks of biomass at the boundary of the region.

249 **2.4.2 Convergence Analysis**

250 To validate the accuracy of the method, convergence analyses on the spatial discretizations will need
 251 to be made. Then the comparison between the semi- and fully-implicit method established in Algo-
 252 rithm 1 can investigated. First, a metric must be formed to enable consistent comparisons between
 253 different simulation solutions. This metric will be referred to as the error.

254 **2.4.2.1 Error Computations**

255 The error is computed by taking the relative normed-difference between two solution in the following
 256 fashion:

257

$$\epsilon_{sol} = \frac{\|u_1 - u_2\|}{\|u_2\|} \quad (2.24)$$

258 where u_1 represents one simulation solution and u_2 represents the solution that is theoretically more
 259 accurate. The theoretical accuracy of u_2 derives from the fact that most comparisons will be done
 260 between solutions that vary in only Δx or between semi- and fully- implicit. These are understood to
 261 have the relation that a smaller Δx , and that the fully-implicit method is to be more accurate. There
 262 is an assumption that both u_1 and u_2 have the same number of grid points, so that the difference can
 263 be taken grid-wise.

264 The results of the error computations, named ϵ_{sol} , is a numerical value for the difference between two
 265 solutions. This depends on the norm used during the computations. Here three norms will be used:

266

$$\ell_1 : \|u\|_1 = \sum_{\pi(i,j)}^{nm} |u_{i,j}| \quad (2.25)$$

267

$$\ell_2 : \|u\|_2 = \sqrt{\sum_{\pi(i,j)}^{nm} (u_{i,j})^2} \quad (2.26)$$

269

$$\ell_\infty : \|u\|_\infty = \max_{\substack{i=1,\dots,n \\ j=1,\dots,m}} |u_{i,j}| \quad (2.27)$$

271 These different norms will all be used to create a broader understanding of the error. This creates three
 272 distinct values for ϵ_{sol} , named ϵ_{ℓ_1} , ϵ_{ℓ_2} , and ϵ_{ℓ_∞} ; each named for the norm used during the computation.

273 **2.4.2.2 Grid Size Convergence**

274 To observe the validity of the method, a test on the convergence of solutions based on the spatial
 275 discritization is done. This will involve using the same simulation described in (2.20) due to the
 276 simplicity.

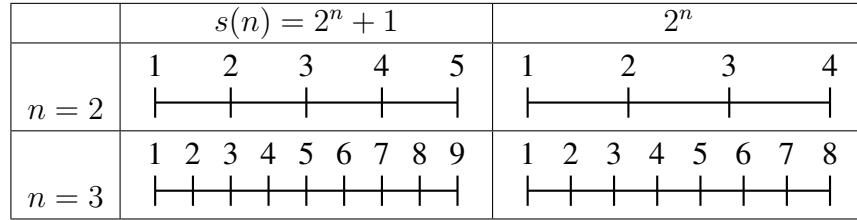


Figure 2.4: Visualization in 1D to illustrate the choice of $s(n) = 2^n + 1$ instead of 2^n for the grid size selection. Here it can be seen that successive grid size selections using $s(n)$ line up on certain grid points and when using 2^n no grid points are equivalent.

277 The convergence will be tracked with only two forms of ϵ_{sol} ; ϵ_1 and ϵ_2 . This is because the value
 278 of ϵ_∞ doesn't vary with the grid size, since the wave front has a steep interface and tends to lead to
 279 inconsistent changes in error. Since the use of ϵ_∞ is not a suitable method for measuring the error, the
 280 inconsistency does not suggest an invalidity with the method. Because of the difference in the number
 281 of grid points between different solutions, u_1 and u_2 , only the grid points in the coarser refinement
 282 will be used. This places a limitation on the selection of grid-sizes since there must be some grid
 283 points locations that are the same for two different chosen grid sizes. For this purpose, we define the
 284 function $s(n) = 2^n + 1$ for $n \in \mathbb{N}$ to be used as the grid size selection function. Now certain grid
 285 points will match without the use of linear interpolation. Here we do not use the typical grid doubling,
 286 2^n , because no grid points equal between two different grid size selection, as illustrated in Figure 2.4.
 287 The results from Figure 2.5 show that the solutions converge as the grid size become refined with the
 288 grid size.

289 2.5 Comparison of Semi-implicit and Fully-implicit Method

290 Here the main comparison that analyses the effects of using Algorithm 1 with different tolerances.
 291 Recall that the main observation is for $tol. = 1$, which correlates to the semi-implicit method since it
 292 will allow only a single iteration of the algorithm.
 293 The simulation used is the same as described in (2.1). The comparison will be on multiple metrics:
 294 the average number of iterations of Algorithm 1, the value of ϵ_1 and ϵ_2 , the computation time of the
 295 simulation, and the location of the wave peak.

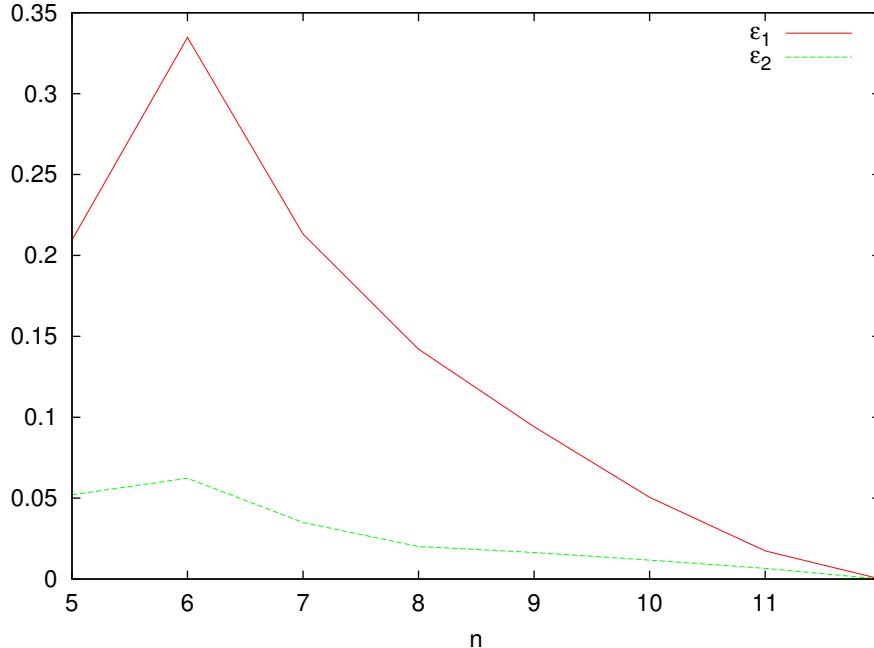


Figure 2.5: Plot showing the convergence of solutions based on changes in Δx . The computations are of ϵ_{ℓ_1} and ϵ_{ℓ_2} with grid-size following $s(n) = 2^n + 1$.

- 296 The average number of iterations are tracked so that an idea of the extra work can be formed. As the
 297 tolerance decreases the amount of iterations the algorithm must perform will increase, the degree of
 298 increase will help relate the amount of work.
- 299 The value of ϵ_1 and ϵ_2 act as a measure of accuracy. Here, these values correspond to the difference be-
 300 tween a pair of solutions, u_1 and u_2 . The (u_1, u_2) pairs are: $(1, 10^{-8})$, $(10^{-8}, 10^{-10})$, $(10^{-10}, 10^{-12})$, $(10^{-12}, 10^{-14})$.
 301 Each row of Table 2.1 refers to the u_1 values of the pairs. Each difference was taken at the last
 302 timestep.
- 303 Along with accuracy, the simulation time is tracked. This is because it represents another metric
 304 for which the viability of the fully-implicit method can be verified. Theoretically there should be a
 305 decrease in the error with the fully-implicit method as the value for tol decreases. Therefore, this
 306 needs to be weighted against the cost of computational intensity and the increase of the simulation
 307 time.
- 308 The location of the wave peak is a tracked quality of the solution that reveals how consistent the
 309 results are. The wave peak is described here as the maximum value of the solution at the final timestep

- 310 calculated. The ultimate goal is that the simulation solutions be converging towards the exact solution.
 311 To see this here the x -coordinate of the wave peak is tracked.

The results of the method comparison can be seen in Table 2.1.

Tol.	Avg. Iter.	ϵ_1	ϵ_2	Time	Wave Peak
1.0e-0	1.00000000	0	0	12.183000000	0.46484375
i.0e-1	1.00000000	0	0	12.208000000	0.46484375
1.0e-2	1.00000000	0	0	12.337999999	0.46484375
1.0e-3	1.00000000	0	0	12.231000000	0.46484375
1.0e-4	1.00000000	0.00200018013	0.000754518705	12.320000000	0.46484375
1.0e-5	1.96505087	2.44746455e-07	1.62832139e-07	18.986999998	0.4609375
1.0e-6	2.00000000	2.81448171e-07	1.94903038e-07	19.091000001	0.4609375
1.0e-7	2.00187495	1.12595285e-05	7.72252591e-06	19.094000001	0.4609375
1.0e-8	2.58568535	7.16665603e-07	1.74044990e-07	20.516999999	0.4609375
1.0e-9	2.90125246	1.05877879e-05	7.00561295e-06	21.308000000	0.4609375
1.0e-10	3.2278443	0.000143911078	9.66349067e-05	22.228000002	0.4609375
1.0e-11	16.099022	4.02028944e-05	2.71613115e-05	57.558999997	0.4609375
1.0e-12	36.318492	4.23049177e-06	2.86249772e-06	113.99400000	0.4609375
1.0e-13	57.681232			173.8489999999999	0.460937500000

Table 2.1: Results from running simulations with different Tol.

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