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Investigating the optimal choice of numerical parameters for solving reaction-diffusion problems with high-order spectral/hp element methods using Nektar++.

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Abstract

Nektar++ is an open-source software package that uses high-order spectral/hp element method to solve a variety of partial differential equations (PDEs). Efficient discretisation allows users to achieve desired solution accuracy with minimal computation time. This paper investigates the optimal choice of element size (h), polynomial order (p), and quadrature point distribution for solving the monodomain equation—a reaction-diffusion PDE—using the CardiacEPSolver in Nektar++ 5.6.0. The results provide guidance for users in configuring parameters in CardiacEPSolver. Findings indicate that the optimal hp combination is sensitive to the mathematical coefficients in the PDE: accuracy improves in more diffusion-dominated processes. Additionally, using electrostatic point distribution reduces runtime but results in poorer solution quality in capturing wavefront geometry compared to Gaussian distribution. To highlight general trends, the data were filtered and interpolated, though this may limit result reliability. Future studies should aim to explore the influence of other parameters in addition to element size and quadrature point and quantify their relationship with the mathematical coefficients of the PDE.

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Contents

List of Figures **ii**

1 Introduction **1**

2 Method **2**
2.1 Problem setup 2
2.2 Experimental methods 2
2.3 Test system 3

3 Results **3**
3.1 Optimal *hp* combination 3
3.2 Changing conductivity and cell membrane capacitance 4
3.3 Comparison of quadrature point distribution 5

4 Discussion **6**

5 Conclusions **6**

References **7**

List of Figures

1 Visualisation (in ParaView 5.11.0) of the solution to the monodomain equation on a rectangular domain showing action potential propagation. The colour bar indicates the voltage from -81.9V to 5V. 1
2 Contour plots showing the runtime (blue dotted line) in seconds and error (red solid line) in conduction speed relative to the true speed in solving the monodomain equation for each *hp* combination using three types of mesh. 3
3 Contour plots showing the runtime (blue dotted line) in seconds and error (red solid line) in conduction speed relative to the true speed in solving the monodomain equation for each *hp* combination using structured triangular mesh with different coefficients of σ and coefficients of membrane capacitance C_m. . . 4
4 Contour plots showing the runtime (blue dotted line) in seconds and the standard deviation (green line) of the x-coordinates of the wavefront in solving the monodomain equation for each *hp* combination using structured and unstructured triangular mesh with Gaussian and Nodal point distributions used in the cell model. 5

1 Introduction

Nektar++ is an open-source software package that uses spectral/hp element method to solve partial differential equations (PDEs). The solvers in the package support PDEs that can be applied to a wide range of areas such as fluid dynamics, structural dynamics and electrophysiology. The demand for low computational cost in almost all industries urges engineers to minimise computation time while maintaining a guaranteed level of accuracy. Compared to the traditional finite element method, spectral/*hp* element method improves solution accuracy by refining both element size (h) and polynomial order (p). Previous studies have shown that the so-called *hp*-refinement converges at an exponential rate, making it more efficient than relying solely on h-type or p-type refinement [1]. However, increasing both h-type and p-type refinement comes at the cost of increased computation time at varying rates. Consequently, determining the optimal combination of *hp* is non-trivial. Furthermore, the optimal *hp* combination is sensitive to the mathematical coefficients in the PDE and changes with the type of PDE to be solved. In addition to polynomial order and mesh element size, the discretisation is governed by a rich set of parameters. The choice of quadrature point distribution is one of them that could impact the accuracy and runtime of the solution. For example, misalignment in unstructured triangular elements and interpolation error can result in poor simulation quality in capturing regular geometries, such as a straight wavefront. In such cases, increasing the polynomial order with Gaussian quadrature point distribution may not improve the solution quality efficiently, due to the computation power not being distributed evenly. An alternative approach could involve using electrostatic point distribution which may offer better performance.

This paper explores the optimal *hp* combination and compares the performance of Gaussian and electrostatic quadrature point distributions for solving two-dimensional reaction-diffusion PDEs using high-order spectral/hp element method. Note that electrostatic distribution is also referred to as nodal distribution and both terms are used interchangeably in this paper. The CardiacEPSolver in Nektar++ was used to solve the monodomain equation as an example, with polynomial order ranging from 2 to 15 at varying mesh sizes on a rectangular domain. A visualisation of the example problem is shown in Figure 1. The aim of this paper is to assist Nektar++ users in selecting optimal parameters for using the CardiacEPSolver.

The setup of the example problem and the experimental method are described in Section 2. Results and findings are presented and limitations are discussed in Section 3 and Section 4. Finally, advice on tuning parameters for the CardiacEPSolver is summarised in Section 5.

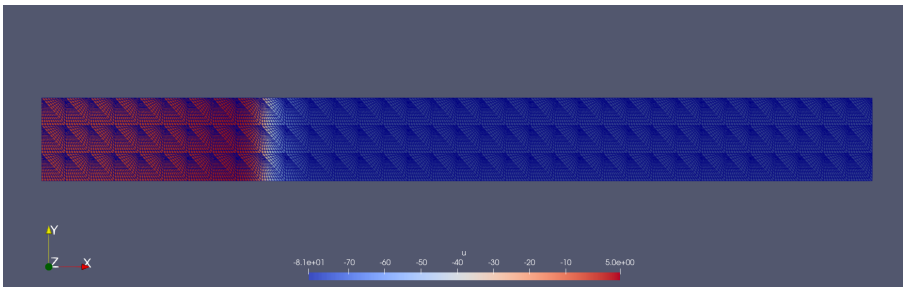


Figure 1: Visualisation (in ParaView 5.11.0) of the solution to the monodomain equation on a rectangular domain showing action potential propagation. The colour bar indicates the voltage from -81.9V to 5V.

2 Method

2.1 Problem setup

The problem considered in this paper is the monodomain equation (Equation 1 [2]) on a rectangular domain $[0, 10][0, 1]$, where σ and C_m represent the coefficient of (isotropic) conductivity and the coefficient of cell membrane capacitance respectively. These two coefficients govern the diffusivity of the solution.

$$\chi[C_m \frac{\partial V_m}{\partial t} + J_{ion}] = \nabla \cdot (\sigma \nabla V_m) \tag{1}$$

For the study of quadrature point, the domain was enlarged to $[0, 10][0, 5]$. The reason for doing so is explained in Section 2.2. The example problem was solved using CardiacEPSolver in Nektar++ 5.6.0.

The monodomain equation models the propagation of action potential (AP) generated by cardiac cells in human heart tissue. Such propagation is governed by both the spatial diffusion of action potential along the tissue and the physical-chemical reactions within the cells. The CardiacEPSolver supports a number of cell models. In this study, the Courtemanche model [3] (called CourtemancheRamirezNattel98 in the software) was used. The solver handles the cell model and the PDE separately using different numerical methods for each. In this paper, we are interested in the choice of quadrature point distribution used in the cell model. To enable nodal distribution, users need to manually modify the C++ source code. The wave propagation was excited by applying a uniform stimulus to a region that covers the left boundary. It is trivial to see that the solution should be constant in the y-direction at any time step, resulting in a uniform wavefront. Simulations were conducted on three types of meshes: structured triangular mesh, unstructured triangular mesh and structured quadrilateral mesh. The meshes were generated using Gmsh 4.8.4.

2.2 Experimental methods

The element size (h) was quantified as the area of the domain divided by the number of elements generated. The ratio between the number of vertices on the x-axis and that on the y-axis was kept the same whenever possible to eliminate the influence of mesh shape on accuracy and runtime, particularly to avoid mesh distortion. The polynomial order studied ranged from 2 to 15, as this range is commonly considered high order in spectral/hp element method [4]. To identify the optimal choice, simulations were run on all hp combinations and their runtime and solution accuracy were compared. The same experiment was repeated with different values of conductivity σ and membrane capacitance C_m to observe how they affect the optimal hp combinations. The conduction speed of the wavefront was used as a metric for solution accuracy. The wavefront was defined as the set of points with the highest voltages at each time step along the horizontal lines that these points lie on. The speed was calculated by measuring the time taken for the wavefront to travel between two fixed history points - a built-in feature supported by the solver. Since the problem does not have an analytical solution, a much finer mesh (with a h that is 7 times smaller than the h of the finest mesh used in other simulations) with a polynomial order of 18 was used to compute an approximated "true" solution. This fine solution was then used to compute the error in conduction speed. The runtime for each simulation was recorded using the solver's built-in function.

As mentioned earlier, the wavefront should be a straight line parallel to the y-axis. The uniformity (or variation) of the wavefront, calculated for both distributions, was used as a measure of solution quality. The uniformity was quantified as the standard deviation of the x-coordinates of the points on the wavefront at each time step. The standard deviation was computed for all time steps and the mean was taken for comparison. Additionally, the width

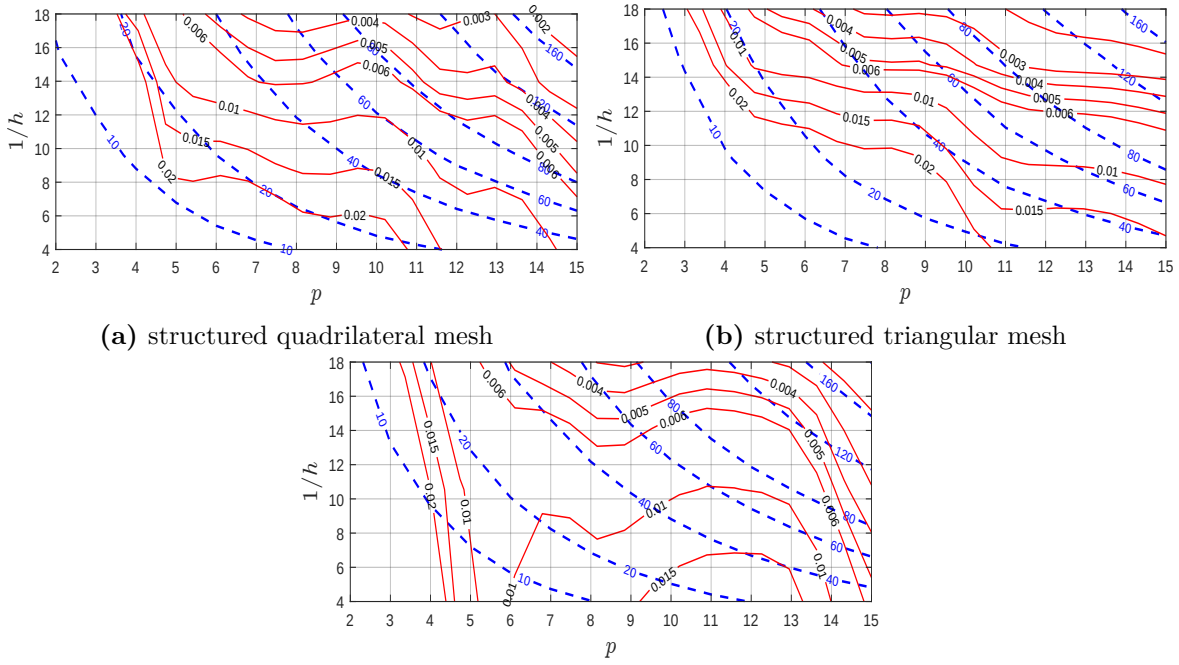
of the domain was increased from 1 to 5 to increase the sample size to highlight the impact of point distribution on the variation of the wavefront.

2.3 Test system

The computation time is highly dependent on the hardware used. In this paper, the study on the optimal *hp* combination was conducted on a 64-bit system with dual 20-core 2.20 GHz Intel Xeon E5-2698 v4 processors and 251 GB of memory. The study on quadrature point choice was conducted on a 64-bit system with a 1.30GHz Intel Core i7-1065G7 processor and 16GB system memory. All visualisations and post-processing of simulation results were carried out using ParaView 5.11.0. The simulations used the implicit-explicit method (called IMEXdirk_3_4_3 in the solver).

3 Results

3.1 Optimal *hp* combination



(a) structured quadrilateral mesh

(b) structured triangular mesh

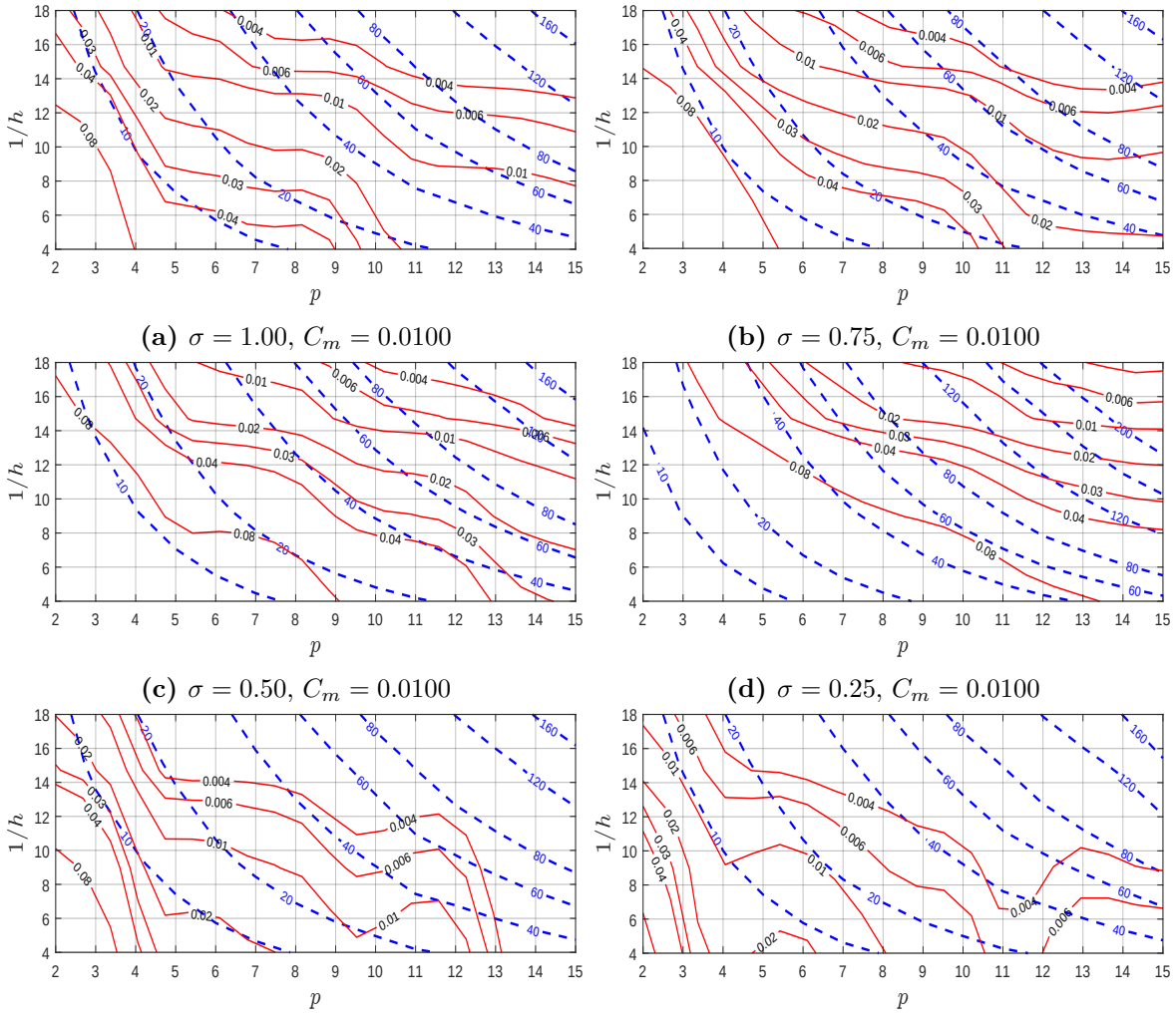
(c) unstructured triangular mesh

Figure 2: Contour plots showing the runtime (blue dotted line) in seconds and error (red solid line) in conduction speed relative to the true speed in solving the monodomain equation for each *hp* combination using three types of mesh.

The optimal *hp* combination was defined as the one that gives the shortest runtime for a desired level of error. Figure 2 can be used as a reference for selecting the optimal discretisation. The inverse of h on the y-axis effectively reflects the number of elements generated. In general, increasing the polynomial order above 6 yields a reduced effect on improving the accuracy. This is particularly evident when the number of elements is high (around $1/h = 18$), where increasing the polynomial order becomes more effective than refining the mesh. This trend holds true for all three types of mesh used. Additionally, some error contours do not intersect the x-axis, indicating a minimum element size required to achieve certain levels of accuracy. For example, achieving an error smaller than 0.6% using structured quadrilateral mesh requires an element size smaller than 1/7. The structured triangular mesh reaches errors below 0.3% more

efficiently than the other two types in this specific example. Runtime remained consistent across mesh types. It should be noted that the data in Figure 2 has been filtered and interpolated to highlight general trends more clearly. While minimal filtering and interpolation were applied consistently, it is possible that individual cases may deviate significantly from the observed trend, such as the singular case at around $p = 5$ and $1/h$ between 4 and 12 with unstructured triangular mesh. This case deviates from the trend observed in the structured meshes and was not filtered out. Also, with quadrilateral and unstructured triangular mesh, there is a sharp increase in accuracy from $p = 14$ to $p = 15$. This suggests that the simulation may be sensitive to the polynomial order such that the accuracy is much higher at some specific orders.

3.2 Changing conductivity and cell membrane capacitance



(a) $\sigma = 1.00$, $C_m = 0.0100$ **(b)** $\sigma = 0.75$, $C_m = 0.0100$

(c) $\sigma = 0.50$, $C_m = 0.0100$ **(d)** $\sigma = 0.25$, $C_m = 0.0100$

(e) $\sigma = 0.10$, $C_m = 0.0050$ **(f)** $\sigma = 0.10$, $C_m = 0.0025$

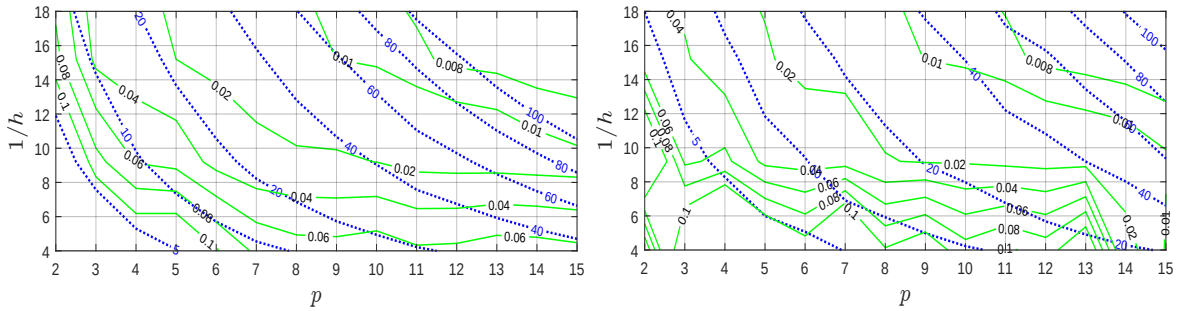
Figure 3: Contour plots showing the runtime (blue dotted line) in seconds and error (red solid line) in conduction speed relative to the true speed in solving the monodomain equation for each hp combination using structured triangular mesh with different coefficients of σ and coefficients of membrane capacitance C_m.

In summary, both decreasing the conductivity and increasing the membrane capacitance can increase the error without affecting runtime. The effects of these parameters can be understood by inspecting Equation 1.

Figure 3 compares the error and runtime for each hp combination using structured triangular mesh with different σ and C_m. Notice that all the plots in Figure 3 have the same values of errors and runtime plotted. Figures 3a to 3d show that decreasing the conductivity generally

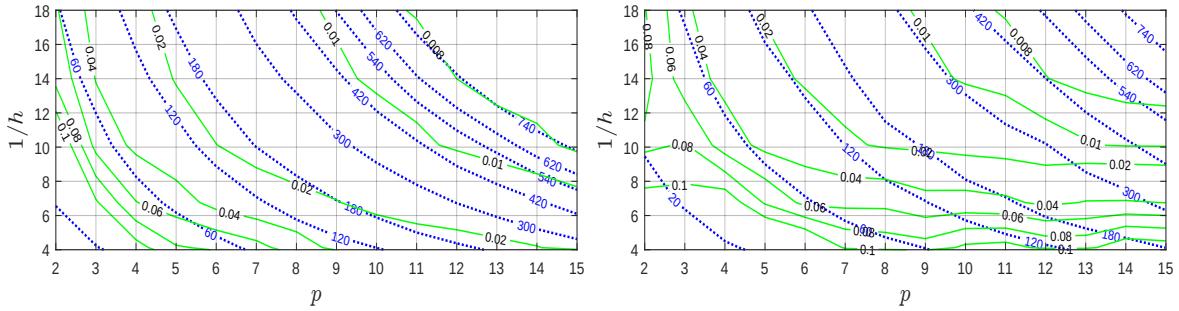
pushes the error contours further up and to the right but preserves their shapes, with the runtime contours being the same. A similar trend can be observed with increasing values of the membrane capacitance as shown in Figures 3a, 3e and 3f. As with the previous section, the error plots have been filtered and interpolated to emphasize overall trends rather than specific hp combinations.

3.3 Comparison of quadrature point distribution



(a) Structured triangular mesh, Gaussian distribution

(b) Structured triangular mesh, Nodal distribution



(c) Unstructured triangular mesh, Gaussian distribution

(d) Unstructured triangular mesh, Nodal distribution

Figure 4: Contour plots showing the runtime (blue dotted line) in seconds and the standard deviation (green line) of the x-coordinates of the wavefront in solving the monodomain equation for each hp combination using structured and unstructured triangular mesh with Gaussian and Nodal point distributions used in the cell model.

Switching from Gaussian to nodal quadrature points significantly reduces runtime, as expected, since nodal distribution uses fewer quadrature points. However, this comes at the cost of reduced solution quality, particularly in terms of capturing the uniformity of the wavefront. Figures 4a and 4b show that increasing the polynomial order or the number of elements consistently improves wavefront uniformity for both Gaussian and nodal distributions.

In the case of unstructured triangular mesh, where the domain was enlarged to [0,10][0,5], Figures 4c and 4d reveal that nodal distribution generally results in poorer uniformity compared to Gaussian distribution, except for cases where $h > 700$. For large h, both distributions perform similarly. It is also evident that at lower h values, increasing the polynomial order has minimal effect on improving uniformity when using nodal distribution. Nevertheless, using nodal distribution significantly reduces the runtime. Note that Figure 4 was plotted using the original data without being filtered or interpolated.

4 Discussion

The contour plots presented in this paper show the general trends. However, they may not accurately reflect singular cases. For example, Figure 2c demonstrates an unexpected accuracy spike at specific polynomial orders, despite the overall expectation that higher polynomial orders should yield better accuracy, assuming other parameters remain constant. The CardiacEPSolver handles the cell model and the PDE separately using different numerical methods featuring different computation times and errors. Because of this, depending on whether the diffusion or the reaction process dominates the propagation, which is determined by the numerical values in the monodomain equation, the optimal *hp* combination for a desired accuracy may vary. As indicated in Figure 3, error reduction tends to occur when the PDE is more diffusion-dominated. The reduction in runtime with nodal point distribution was anticipated, as nodal distribution uses fewer nodes compared to Gaussian distribution. However, this reduction comes at the cost of solution quality, particularly in terms of capturing the uniformity of the wavefront, as shown in Figures 4a and 4b. While nodal distribution might offer a performance advantage, its impact on accuracy should be carefully considered, especially in cases where the precision of the geometry is important.

Limitations in this study are recognised. Firstly, the reliability of the results is affected by the filtering and interpolation applied to the data. More refined simulations with finer incremental steps in h could have reduced the need for interpolation, providing a clearer representation of trends. Moreover, alternative methods for error computation should be explored to minimise bias and improve the accuracy of general trend identification. One potential improvement could be utilising the built-in interpolation feature in Nektar++ to map the fine solution onto the coarse discretisation's solution field and compute the $L2$ error directly. Secondly, the unstructured triangular mesh used in this study still displayed some degree of orderliness due to the rectangular geometry of the domain. As a result, the findings may not fully generalise to truly unstructured mesh configurations. Future work should explore more complex geometries to assess the robustness of the methods. Thirdly, the code for nodal distribution is still under development and has not been rigorously tested for its functionality. Further validation is needed to ensure its accuracy and reliability. Additionally, nodal distribution should be tested under varying mathematical coefficients in the PDE to better understand its impact on the optimal *hp* combination. For example, by using a more reaction-dominated PDE, the effects of nodal distribution on solving the cell model may become more pronounced. This would allow for a more comprehensive assessment of how the mathematical coefficients influence the performance of different *hp* combinations.

5 Conclusions

It is important to emphasise that the dicretisation is governed by a number of numerical parameters and the optimal choice is sensitive to the nature of the PDE. This paper only explores the tuning of element size (h) and polynomial order (p) for solving reaction-diffusion PDE at varying conductivities and with Gaussian and electrostatic quadrature point distributions.

Among the three types of mesh tested, the unstructured triangular mesh is likely of most interest to users, as it better captures complex geometries compared to structured meshes. The optimal *hp* combination ultimately depends on the desired level of accuracy. In general, increasing either the number of elements or the polynomial order leads to longer computation times. However, increasing the polynomial order beyond 7, or increasing the number of elements beyond $1/h = 14$, offers diminishing returns in terms of accuracy improvement. Additionally, a minimum number of elements is sometimes required, regardless of the polynomial order, to achieve a given accuracy. The contour plots presented in this paper can be directly referenced

to guide users in selecting the appropriate discretization based on the conductivity and their specific accuracy and runtime requirements. For problems with lower conductivity—where the process is more diffusion-dominated—users should consider employing a finer mesh with a higher polynomial order to maintain accuracy, as indicated by the trends in Figure 3. When selecting a quadrature point distribution for the cell model, using electrostatic (nodal) distribution can significantly reduce runtime, but it may lead to reduced solution quality, particularly in capturing the wavefront. As the nodal distribution code in Nektar++ 5.6.0 has not been extensively tested, its use is not recommended at this time.

Future studies should aim to explore the influence of other parameters on runtime and accuracy to further clarify and quantify the relationship between the optimal discretisation choices and the mathematical coefficients of the PDE.

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