

Meshless Method for Solving Coupled Nonlinear Reaction-Diffusion  
Equations Using Moving Kriging Approximation

Miss Kanittha Yimnak M.Sc. (Applied Statistics)

A Dissertation Submitted in Partial Fulfillment of the Requirements  
for the Degree of Doctor of Philosophy (Applied Mathematics)  
Faculty of Science  
King Mongkut's University of Technology Thonburi  
2014

Dissertation Committee

..... Chairman of Dissertation Committee  
(Asst. Prof. Surattana Sungnul, Ph.D.)

..... Member and Dissertation Advisor  
(Asst. Prof. Anirut Luadsong, Ph.D.)

..... Member  
(Asst. Prof. Sumlearng Chunrungsikul, Ph.D.)

..... Member  
(Assoc. Prof. Settapat Chinviriyasit, Ph.D.)

Dissertation Title	Meshless Method for Solving Coupled Nonlinear Reaction-Diffusion Equations Using Moving Kriging Approximation
Dissertation Credits	36
Candidate	Miss Kanittha Yimnak
Dissertation Advisor	Asst. Prof. Dr. Anirut Luadsong
Program	Doctor of Philosophy
Field of Study	Applied Mathematics
Department	Mathematics
Faculty	Science
Academic Year	2014

### ABSTRACT

In this research, the meshless local Pretrov-Galerkin method with the test function in view of the Heaviside step function is developed to solve the system of coupled nonlinear reaction-diffusion equations in two dimensional spaces subjected to Dirichlet and Neumann boundary conditions on a square domain. Two-field velocities are approximated by moving Kriging approximation for constructing nodal shape function that holds the Kronecker delta property, thereby enhancing the arrangement nodal shape construction accuracy while the Euler, Runge-Kutta and Crank-Nicolson methods are chosen for temporal discretization. For the Crank-Nicolson method, the nonlinear terms are treated iteratively within each time step. The developed formulation is verified in two numerical examples with investigations on the convergence and the accuracy of numerical results. The numerical experiments reveal the solutions using the developed formulation which are stable and more precise.

Keywords : Crank-Nicolson Method / Euler Method / Meshless Local Pretrov-Galerkin Method / Moving Kriging Approximation / Reaction-Diffusion Equations / Runge-Kutta Method

หัวข้อวิทยานิพนธ์	วิธีเมซเลสสำหรับการแก้ปัญหาสมการการแพร่ปฏิกิริยาเคมีที่ไม่เป็นเชิงเส้นแบบคู่โดยการใชตัวประมาณแบบมูฟวี่งคริกกิง
หน่วยกิต	36
ผู้เขียน	นางสาวกนิษฐา ยี่มนาค
อาจารย์ที่ปรึกษา	ผศ. ดร. อนิรุทธ ลวดทรง
หลักสูตร	ปรัชญาคุษฎีบัณฑิต
สาขาวิชา	คณิตศาสตร์ประยุกต์
ภาควิชา	คณิตศาสตร์
คณะ	วิทยาศาสตร์
ปีการศึกษา	2557

#### บทคัดย่อ

วิทยานิพนธ์นี้นำเสนอการพัฒนาวิธีเมซเลสโลคัลฟิทรอฟ-กาเลอคินกับการใช้ฟังก์ชันทดสอบแบบฟังก์ชันเฮฟวีไซด์สเต็ป เพื่อใช้ในการแก้ปัญหาสมการการแพร่ปฏิกิริยาเคมีที่ไม่เป็นเชิงเส้นแบบคู่ใน 2 มิติภายใต้เงื่อนไขขอบเขตแบบดิริคเล และนอยมันน์ ในโดเมนที่มีลักษณะเป็นแบบสี่เหลี่ยม สำหรับในขั้นตอนการสร้างฟังก์ชันรูปร่างเพื่อประมาณค่าตัวแปรที่เกี่ยวกับความเร็วทั้งสองตัวแปรจะทำการประมาณค่าโดยวิธีมูฟวี่งคริกกิง ทั้งนี้เนื่องจากวิธีมูฟวี่งคริกกิงมีคุณสมบัติฟังก์ชันเดลตาโครเนกเกอร์ ซึ่งคุณสมบัติดังกล่าวมีส่วนช่วยในการเพิ่มความแม่นยำในการประมาณค่าตัวแปรที่เกี่ยวกับความเร็วในส่วนของการประมาณค่าแบบไม่ต่อเนื่องเชิงเวลา ในวิทยานิพนธ์นี้จะประยุกต์ใช้ ทั้งวิธีออยเลอร์ วิธีรุงเงอ-คุททา และ วิธีแรงคั่นโคลสัน โดยสำหรับวิธีแรงคั่นโคลสันนี้จะคำนวณพจน์ของสมการที่ไม่เป็นเชิงเส้นด้วยวิธีทำซ้ำในแต่ละขั้นของเวลา และวิธีที่พัฒนาขึ้นนี้จะนำไปประยุกต์ใช้ในสองตัวอย่างเพื่อตรวจสอบการลู่เข้าและความถูกต้องของผลลัพธ์ในเชิงตัวเลข ซึ่งจากผลการทดลองแสดงให้เห็นว่าวิธีที่พัฒนาขึ้นมานี้มีความเสถียรและแม่นยำในการแก้ปัญหาดังกล่าว

คำสำคัญ : ตัวประมาณมูฟวี่งคริกกิง / วิธีแรงคั่นโคลสัน / วิธีเมซเลสโลคัลฟิทรอฟ-กาเลอคิน / วิธีรุงเงอ-คุททา / วิธีออยเลอร์ / สมการการแพร่ปฏิกิริยาเคมี

## **ACKNOWLEDGEMENTS**

This dissertation has been completed because of suggestion from the a state-of-the-art technical computing language and numerical algorithms by Asst.Prof.Dr. Anirut Luadsong who is my advisor. I would like to express appreciation for his kindness. In addition, I would like to show my gratitude towards Asst. Prof. Surattana Sungnul, the chairman of the dissertation committee, who shared her valuable time with her thoughtful comments. I also would like to thank Asst. Prof. Dr. Sumlearnng Chunrungsikul and Assoc. Prof. Dr. Settapat Chinviriyasit, who shared their time as my dissertation committee. Moreover, I would like to thank Dhurakij Pundit University for the scholarship and their financial support.

Finally, I would like to thank my family and friends in King Mongkut's University of Technology Thonburi, for encouragement.

## CONTENTS

	PAGE
ENGLISH ABSTRACT	ii
THAI ABSTRACT	iii
ACKNOWLEDGEMENTS	iv
CONTENTS	v
LIST OF TABLES	vii
LIST OF FIGURES	viii
LIST OF TECHNICAL VOCABULARY AND ABBREVIATIONS	xi
 <b>CHAPTER</b>	
<b>1. INTRODUCTION</b>	<b>1</b>
1.1 Rationale	1
1.2 Literature Review	2
1.3 Objective of Research	5
1.4 Scope of Research	5
1.5 Advantage of Research	5
 <b>2. THEORETICAL BACKGROUND</b>	<b>6</b>
2.1 Governing Equation	6
2.2 Brusselator System	6
2.3 Constructing Shape Function	7
2.3.1 Moving Kriging Approximation	7
2.3.2 Radial Point Interpolation Method	10
2.4 Test Function	12
2.4.1 The fundamental solution	12
2.4.2 The Heaviside Step Function	13
2.5 Numerical Method	13
2.5.1 Trapezoidal Rule	13
2.5.2 Simpson Rule	14
2.5.3 Midpoint Rule	15
2.5.4 Gauss-Legendre Quadrature Method	16
2.6 Temporal Discretization	19
2.6.1 Euler Method	19
2.6.2 Runge-Kutta Method	19
2.6.3 Crank-Nicolson Method	20
 <b>3. METHODOLOGY</b>	<b>22</b>
3.1 Space Discretization by MLPG Method with a Heaviside Step Test Function (MLPG5)	22
3.2 Space Discretization by MLPG Method with The Fundamental Solution Test Function (MLPG4)	26

	<b>PAGE</b>
<b>4. NUMERICAL EXPERIMENTS</b>	<b>32</b>
4.1 Example 1	32
4.1.1 The Results of Example 1 by MLPG5 Method Based on MKA	34
4.1.2 The Results of Example 1 by The MLPG5 Method Based on RPIM	40
4.1.3 The Results of Example 1 by The MLPG4 Method Based on MKA	44
4.2 Example 2, application for Brusselator system	45
4.2.1 The Results of Example 2 by The MLPG5 Method Based on MKA	46
4.2.2 The Results of Example 2 by The MLPG5 Method Based on RPIM	49
<b>5. CONCLUSIONS AND RECOMMENDATIONS</b>	<b>52</b>
5.1 Conclusions	52
5.2 Recommendations	52
<b>REFERENCES</b>	<b>53</b>
<b>BIOGRAPHY</b>	<b>55</b>

## LIST OF TABLES

TABLE	PAGE
2.1 Abscissas and weights for Gaussian quadrature.	18
4.1 The solution by the MLPG5 method based on MKA and using $m = 10, N = 441$ and $\Delta t = 0.1$ obtained at some different points.	46
4.2 The solution by the MLPG5 method based on RPIM and using $m = 10, N = 441$ and $\Delta t = 0.1$ obtained at some different points.	49

## LIST OF FIGURES

FIGURE	PAGE
2.1 Local boundaries, the supports of nodes , the domain of definition of the MLS approximation for the trial function at a point.	13
2.2 Geometric representation.	14
2.3 Simpson's rule can be derived by approximating the integrand $f(x)$ by the quadratic interpolant $P(x)$ .	15
2.4 Midpoint approximation.	16
2.5 The Crank–Nicolson stencil for a 1-D problem.	21
4.1 Both error of $u$ and $v$ using the MKA with temporal discretization by the Euler method and $\Delta t = 0.01$ : (a) MRE of $u$ ; (b) MRE of $v$ ; (c) RMSRE of $u$ ; (d) RMSRE of $v$ .	34
4.2 Both error of $u$ and $v$ using the MKA with temporal discretization by the Runge-Kutta method and $\Delta t = 0.01$ : (a) MRE of $u$ ; (b) MRE of $v$ ; (c) RMSRE of $u$ ; (d) RMSRE of $v$ .	35
4.3 Both error of $u$ and $v$ using the MKA with temporal discretization by the Crank-Nicolson method and $\Delta t = 0.01$ : (a) MRE of $u$ ; (b) MRE of $v$ ; (c) RMSRE of $u$ ; (d) RMSRE of $v$ .	35
4.4 The comparison of MRE of $u$ and $v$ based on the MKA among the Euler, Runge-Kutta and Crank-Nicolson methods, $m = 10, t = 0.1$ and $\Delta t = 0.01$ : (a) MRE of $u$ ; (b) MRE of $v$ .	36
4.5 The comparison of RMSRE of $u$ and $v$ based on the MKA among the Euler, Runge-Kutta and Crank-Nicolson methods, $m = 10, t = 0.1$ and $\Delta t = 0.01$ : (a) RMSRE of $u$ ; (b) RMSRE of $v$ .	36
4.6 Exact solutions of $u$ and $v$ using $N=441, m = 10, t = 0.1$ and $\Delta t = 0.01$ : (a) exact solution of $u$ ; (b) exact solution of $v$ .	36
4.7 Trial solutions and errors of $u$ and $v$ by the MLPG5 method based on MKA with temporal discretization by the Euler method, $N=441, m = 10, t = 0.1$ and $\Delta t = 0.01$ : (a) trial solution of $u$ ; (b) corresponding error profile of $u$ ; (c) trial solution of $v$ ; (d) corresponding error profile of $v$ .	37
4.8 Trial solutions and errors of $u$ and $v$ by the MLPG5 method based on MKA with temporal discretization by the Runge-Kutta method, $N = 441, m = 10, t = 0.1$ and $\Delta t = 0.01$ : (a) trial solution of $u$ ; (b) corresponding error profile of $u$ ; (c) trial solution of $v$ ; (d) corresponding error profile of $v$ .	38
4.9 Trial solutions and errors of $u$ and $v$ by the MLPG5 method based on MKA with temporal discretization by the Crank-Nicolson method, $N = 441, m = 10, t = 0.1$ and $\Delta t = 0.01$ : (a) trial solution of $u$ ; (b) corresponding error profile of $u$ ; (c) trial solution of $v$ ; (d) corresponding error profile of $v$ .	38

## LIST OF FIGURES (Cont.)

FIGURE	PAGE
4.10 Both errors of $u$ and $v$ by the MLPG5 method based on MKA with temporal discretization by the Crank-Nicolson methods against the number of nodal points, $m = 10, t = 1$ and $\Delta t = 0.1$ : (a) MRE of $u$ and $v$ ; (b) RMSRE of $u$ and $v$ .	39
4.11 Exact solutions of $u$ and $v$ using $N = 441, m = 10, t = 1$ and $\Delta t = 0.1$ : (a) exact solution of $u$ ; (b) exact solution of $v$ .	39
4.12 Trial solutions and errors of $u$ and $v$ by the MLPG5 method based on MKA with temporal discretization by the Crank-Nicolson methods, $N=441, m = 10, t = 1$ and $\Delta t = 0.1$ : (a) trial solution of $u$ ; (b) corresponding error profile of $u$ ; (c) trial solution of $v$ ; (d) corresponding error profile of $v$ .	40
4.13 Both error of $u$ and $v$ by the MLPG5 method based on the RPIM with temporal discretization by the Runge-Kutta method and $\Delta t = 0.01$ : (a) MRE of $u$ ; (b) MRE of $v$ ; (c) RMSRE of $u$ ; (d) RMSRE of $v$ .	40
4.14 Both error of $u$ and $v$ the MLPG5 method based on the RPIM with temporal discretization by the Crank-Nicolson method and $\Delta t = 0.01$ : (a) MRE of $u$ ; (b) MRE of $v$ ; (c) RMSRE of $u$ ; (d) RMSRE of $v$ .	41
4.15 Both error of $u$ and $v$ by the MLPG5 method based on the RPIM with temporal discretization by the Crank-Nicolson method and $\Delta t = 0.1$ : (a) MRE of $u$ ; (b) MRE of $v$ ; (c) RMSRE of $u$ ; (d) RMSRE of $v$ .	42
4.16 Trial solutions and errors of $u$ and $v$ by the MLPG5 method based on the RPIM with temporal discretization by the Runge-Kutta method, $N = 441, m = 10, t = 0.1$ and $\Delta t = 0.01$ : (a) trial solution of $u$ ; (b) corresponding error profile of $u$ ; (c) trial solution of $v$ ; (d) corresponding error profile of $v$ .	42
4.17 Trial solutions and errors of $u$ and $v$ by the MLPG5 method based on the RPIM with temporal discretization by the Crank-Nicolson method, $N = 441, m = 10, t = 0.1$ and $\Delta t = 0.01$ : (a) trial solution of $u$ ; (b) corresponding error profile of $u$ ; (c) trial solution of $v$ ; (d) corresponding error profile of $v$ .	43
4.18 Trial solutions and errors of $u$ and $v$ by the MLPG5 method based on the RPIM with temporal discretization by the Crank-Nicolson method, $N = 441, m = 10, t = 1$ and $\Delta t = 0.1$ : (a) trial solution of $u$ ; (b) corresponding error profile of $u$ ; (c) trial solution of $v$ ; (d) corresponding error profile of $v$ .	44
4.19 Trial solutions and errors of $u$ and $v$ by MLPG4 method based on MKA against the number of nodal points at time instant $t = 0.1$ using $\Delta t=0.01$ and $N = 441$ : (a) RMSRE of $u$ and $v$ ; (b) trial solution of $u$ ; (c) corresponding error profile of $u$ ; (d) trial solution of $v$ ; (e) corresponding error profile of $v$ .	45

## LIST OF FIGURES (Cont.)

FIGURE	PAGE
4.20 Concentration profiles of $u$ and $v$ : (a) $u$ at $t = 0$ ; (b) $v$ at $t = 0$	47
4.21 The approximate solutions of $u$ and $v$ at $t = 10$ obtained by the MLPG5 method based on MKA using $N = 441, m = 10$ and $\Delta t = 0.1$ : (a) $u$ using the Euler method; (b) $v$ using the Euler method; (c) $u$ using the Runge-Kutta method; (d) $v$ using the Runge-Kutta method; (e) $u$ using the Crank-Nicolson method; (f) $v$ using the Crank-Nicolson method.	48
4.22 The approximate solutions at $t = 10$ obtained by the MLPG5 method based on RPIM using $N = 441, m = 10$ and $\Delta t = 0.1$ : (a) $u$ using the Runge-Kutta method; (b) $v$ using the Runge-Kutta method; (c) $u$ using the Crank-Nicolson method; (d) $v$ using the Crank-Nicolson method	51

## LIST OF TECHNICAL VOCABULARY AND ABBREVIATIONS

$u, v$	=	two-field velocities
$\mathbb{R}^2$	=	2-dimensional real space
$D_1, D_2$	=	the diffusion coefficients of the chemical species
$\delta$	=	the Kronecker delta
$\phi(\mathbf{x}), \Phi(\mathbf{x})$	=	shape function and its vector form
$\Omega$	=	problem domain, plate domain
$\Omega_s^i$	=	local sub-domain
$\partial\Omega_s^i$	=	boundary of local sub-domain
$\Gamma$	=	boundary of domain
$\Gamma_D$	=	essential boundary
$\Gamma_N$	=	natural boundary
$L_s^i$	=	the part of boundary $L_s$ which is inside the global domain
$\Gamma_{SD}^i$	=	the part of overlap between the boundary of the local sub-domain and the essential boundary
$\Gamma_{SN}^i$	=	the part of overlap between the boundary of the local sub-domain and the natural boundary
$\mathbf{n}$	=	the outward unit normal direction to the boundary $\partial\Omega$
$A, B$	=	functions of the field variable $u$ and $v$
$f_1, f_2$	=	functions of prescribed sources
$w$	=	a Heaviside step
$u^*$	=	a fundamental solution
$m$	=	the order of monomial basis
$N$	=	the number of nodes
$p(\mathbf{x}), \mathbf{P}(\mathbf{x})$	=	basis function and its vector form
$\mathbf{A}, \mathbf{B}$	=	coefficients vector form by MKA method
$\gamma(\mathbf{x}), \mathbf{r}(\mathbf{x})$	=	correlation Gaussian function and its vector form
$\mathbf{R}$	=	correlation matrix
$r_{ij}$	=	the distance between point of interest $\mathbf{x}$ and a node $(x_i, y_i)$
$a, \mathbf{a}$	=	coefficients and its vector form by RPIM method
$b, \mathbf{b}$	=	coefficients and its vector form by RPIM method
$R_i(\mathbf{x}), \mathbf{R}_Q$	=	radial basis functions and its vector form by RPIM method
$t$	=	time variable
$\Delta t$	=	time-step
$\theta$	=	correlation parameters
$c$	=	shape-parameter