Convergence of High-Order Deterministic Particle Methods for the Convection-Diffusion Equation

RICARDO CORTEZ
Courant Institute

Abstract

A proof of high-order convergence of three deterministic particle methods for the convection-diffusion equation in two dimensions is presented. The methods are based on discretizations of an integro-differential equation in which an integral operator approximates the diffusion operator. The methods differ in the discretization of this operator. The conditions for convergence imposed on the kernel that defines the integral operator include moment conditions and a condition on the kernel's Fourier transform. Explicit formulae for kernels that satisfy these conditions to arbitrary order are presented. © 1997 John Wiley & Sons, Inc.

1 Introduction

In this paper we present an L^2-convergence proof of high-order deterministic particle methods for the convection-diffusion equation

$$\frac{\partial \Gamma}{\partial t} + (\mathbf{u} \cdot \nabla)\Gamma = \nu \Delta \Gamma \,, \qquad \nabla \cdot \mathbf{u} = 0 \,, \tag{1.1}$$

$$\Gamma(\mathbf{x}, 0) = \Gamma_0(\mathbf{x}) \,, \qquad \mathbf{x} \in \mathbb{R}^2, \tag{1.2}$$

where $\mathbf{u}(\mathbf{x}, t)$ is a prescribed flow and Γ is the solution of the linear equation (1.1) with initial data Γ_0. We discuss the convergence of the particle strength exchange (PSE) method studied by Degond and Mas-Gallic [7] and two other numerical methods that are variants of PSE. The three methods are discretizations of an equation in which the Laplacian is replaced by an integral operator of the type

$$Q\Gamma(\mathbf{x}) = \frac{1}{\sigma^2} \int [\Gamma(\mathbf{y}) - \Gamma(\mathbf{x})] \; \Lambda_\sigma(\mathbf{y} - \mathbf{x}) d\mathbf{y} \,, \tag{1.3}$$

where σ is a numerical parameter and the kernel Λ_σ satisfies appropriate moment conditions. We use the operator in equation (1.3) and properties of the kernel Λ_σ to define three discrete versions of Q that lead to the three numerical methods. They all require the choice of the diffusion kernel in Q. The third method also requires a cutoff function f_δ that must satisfy a condition relating

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f_δ to the kernel Λ_σ. We formulate the precise condition in terms of the Fourier transforms of the two functions in Section 4.

The PSE method for the convection-diffusion equation results from a very natural discretization of equation (1.3). This method has been shown to converge in L^∞ for the case when the kernel of the integral operator is nonnegative [7]. This case is limited to second-order convergence since the moment conditions required for high-order convergence cannot be satisfied by a nonnegative kernel. Further work presented in [7] is restricted to the case when the viscosity ν and the parameter σ satisfy the constraint $\nu \le C\sigma^2$, where C is a constant. This constraint is used to develop bounds for the error in the numerical solution for fixed numerical parameters. However, this constraint represents a serious obstacle to convergence since the limiting case of vanishing numerical parameters cannot be reached.

Our results extend the previous work by presenting the convergence of the PSE method without assuming any dependence of the numerical parameter σ on the viscosity and without the restriction that the kernel be positive. Instead, we require that the Fourier transform of the kernel Λ_σ satisfy $\hat{\Lambda}_\sigma(\mathbf{s}) \le \hat{\Lambda}_\sigma(0)$. This allows the use of high-order kernels leading to acceptable error estimates even for moderate values of viscosity. We also provide examples of kernels of arbitrary order constructed in ways analogous to those in [1].

The main result states that the difference between the numerical solution, Γ_h, and the solution Γ of the convection-diffusion equation satisfies the discrete L^2-norm error estimate

$$\|\Gamma_h - \Gamma\|_{0,2,h} \le C\nu \left(\sigma^d + \frac{h^m}{\sigma^{m+2}} + \frac{h^{m+3/2}}{\sigma^{m+5}} \right),$$

where h is the initial interparticle distance and C is a constant independent of ν and the numerical parameters. The parameter σ must be larger than h but small enough so that the terms in the error bound balance. The exponent m is determined by the smoothness of the flow and initial conditions, while d is the order of the approximation of the Laplacian by the operator Q. High-order kernels yield large values of d and therefore smaller regularization error.

One can exploit further the symmetry of the kernel Λ_σ to arrive at a slightly different discretization of Q. This leads to the first variant (method B) of the PSE method. The main difference between the two methods is that high-order convergence of method B is achieved by requiring that $\nu h^m/\sigma^{m+2} \le 1$. At first glance this condition appears equivalent to the one used in [7]; however, there is an important difference. For given flow properties, the numerical parameters h and σ can be chosen so that this condition is satisfied in the limit as $h, \sigma \to 0$.

A third method (method C) follows from another change in the discretization of the operator Q. We show the convergence of this method under the same assumptions as the PSE method plus one additional condition. This condition is not a very restrictive one and states roughly that the Fourier transform of Λ_σ (normalized by its value at the origin) must be bounded above by the (normalized) Fourier transform of a cutoff function f_δ, which is required in the method. Examples of such functions are given in the last section.

Fishelov [8, 9] introduced a related method in which the Laplacian of the vorticity is approximated by the convolution of the vorticity and the Laplacian of a cutoff function. Convergence in L^2 of this method for the convection-diffusion equation has been established [9]. We show that Fishelov's method is equivalent to method C, and therefore the former can be viewed as a discretization of the integro-differential equation on which the PSE method is based.

The dynamics of physical quantities such as chemical concentrations advected by the flow $\mathbf{u}$ are modeled by equation (1.1). Particle methods for the simulation of incompressible flows are of particular interest in the case of slightly viscous fluids, when other methods can develop stability problems. The PSE and Fishelov's methods have been used in conjunction with vortex methods for the simulation of viscous flows. For example, Bernard [2] adapted Fishelov's method for use within boundary layers, and Winckelmans and Leonard [15] computed the reconnection of two vortex rings in three dimensions using the PSE method. In applications, these methods are commonly used with high-order kernels. We note that the convergence of these methods to solutions of the Navier-Stokes equations has not been established.

In practice, these particle methods sometimes suffer from errors derived from the limit on the size of the discretized domain and from clustering of particles. Although these issues are not addressed in this paper, there is work dedicated to the analysis and reduction of these errors. The size of the domain where the initial particles are placed is often estimated from the final time of the specific simulation. Cottet [5] has made a study of the large-time behavior of the PSE method (with high-order kernel) for the vorticity formulation of Navier-Stokes in two dimensions. He proved that the numerical solution exhibits the same decay rate (of enstrophy) as the solution of the continuous problem for large times. He revealed a useful way to deal with the numerical domain boundary. Sometimes particles tend to form clusters even in incompressible flow applications. Regridding procedures are then required to carry the computation beyond this time and new errors are introduced. Regridding algorithms specifically designed for the PSE or Fishelov's method have been proposed in [4] and [11]. Nordmark has managed to design *rezoning* procedures for use with Fishelov's method that preserve high accuracy.

Finally, we mention other deterministic methods for viscous flows that model the diffusion process by redistributing the vorticity carried by the particles. The method adopted by Cottet and Mas-Gallic [6] and Choquin and Huberson [3] uses viscous splitting and the discrete convolution of the convected vorticity with the heat kernel. A new method of vorticity exchange was recently proposed by Shankar and van Dommelen [13]. In this method the fractions of circulation exchanged among particles are given by the solution of a linear system of equations that is solved at every step.

In the next section of the paper we present the integro-differential equation on which the methods are based, define the kernel Λ_σ and its properties, and introduce the numerical methods. The rest of the paper is divided into three parts. In Section 3 we discuss properties of the solution of the integro-differential equation and present results that show the convergence of this solution to solutions of the convection-diffusion equation. In Section 4 we state and prove the convergence theorem of the PSE method first and then state the corresponding theorems for the other two numerical methods. In the final section we present a discussion and examples of high-order kernels.

1.1 Preliminaries and Notation

Throughout this paper we use the following definitions and notation.

1. For $f \in L^2(\mathbb{R}^2)$, the Fourier transform is defined by

$$\hat{f}(\mathbf{s}) = \frac{1}{2\pi} \int_{\mathbb{R}^2} f(\mathbf{x}) e^{-i\mathbf{s}\cdot\mathbf{x}}\, d\mathbf{x}\,.$$

   With this convention we have that $\widehat{(f * g)} = 2\pi \hat{f}\hat{g}$.

2. Let $p \in [1, \infty)$ and $m \geq 0$. Define the Sobolev space

$$W^{m,p}(\mathbb{R}^2) = \{f : \mathbb{R}^2 \to \mathbb{R} \mid \partial^\beta f \in L^p(\mathbb{R}^2),\ |\beta| \leq m\}$$

   and the norm in $W^{m,p}(\mathbb{R}^2)$,

$$\|f\|_{m,p}^p = \sum_{0 \leq |\beta| \leq m} \|\partial^\beta f\|_{L^p(\mathbb{R}^2)}^p\,.$$

   For $W^{m,\infty}(\mathbb{R}^2)$, we use

$$\|f\|_{m,\infty} = \max_{0 \leq |\beta| \leq m} \|\partial^\beta f\|_{L^\infty(\mathbb{R}^2)}\,.$$

3. A discrete norm is defined by

$$\|f\|_{0,2,h}^2 = \sum_i h^2 \, [f(\mathbf{x}^i)]^2 \,.$$

4. Minkowski's (triangle) inequality states that (see [14], p. 24)

$$\left\| \int f(\cdot,t)dt \right\|_{0,2} \leq \int \|f(\cdot,t)\|_{0,2} \, dt \,.$$

In this paper we assume that $\mathbf{u}(\mathbf{x},t) : \mathbb{R}^2 \times \mathbb{R} \to \mathbb{R}^2$ is a given flow, and we discuss solutions of equation (1.1) and equation (2.1) for $(\mathbf{x},t) \in \mathbb{R}^2 \times [0,T]$ for some positive final time T. We use the notation $L^\infty(0,T;X)$ to denote the space of functions $f : t \to f(t)$ from $(0,T)$ into the Banach space X with norm $\|\cdot\|$ such that

$$\|f\|_{L^\infty(0,T;X)} = \operatorname*{ess\,sup}_{0 \leq t \leq T} \|f(t)\| < +\infty \,.$$

2 The Numerical Methods

The numerical methods presented in this paper are based on discretizations of an integro-differential equation that approximates equation (1.1) by replacing the Laplacian with an integral operator. The integro-differential equation is

$$\frac{\partial \Gamma}{\partial t} + (\mathbf{u} \cdot \nabla)\Gamma = \nu Q \Gamma \,, \qquad \nabla \cdot \mathbf{u} = 0 \,, \tag{2.1}$$

$$\Gamma(\mathbf{x},0) = \Gamma_0(\mathbf{x}) \,, \qquad \mathbf{x} \in \mathbb{R}^2 \,. \tag{2.2}$$

The operator Q is defined by

$$Q\Gamma(\mathbf{x}) = \frac{1}{\sigma^2} \int [\Gamma(\mathbf{y}) - \Gamma(\mathbf{x})] \, \Lambda_\sigma(\mathbf{y}-\mathbf{x}) d\mathbf{y} \,, \tag{2.3}$$

with $\Lambda_\sigma(\mathbf{x}) = \sigma^{-2}\Lambda(|\mathbf{x}|/\sigma)$ and $\Lambda(r)$ a smooth, radially symmetric function that satisfies the following conditions for $2 \leq d$:

(K1) $\int x_i^2 \, \Lambda(|\mathbf{x}|) d\mathbf{x} = 2 \quad$ for $i = 1,2$,

(K2) $\int \mathbf{x}^\beta \, \Lambda(|\mathbf{x}|) d\mathbf{x} = 0 \quad$ for $|\beta| = 1, \; 3 \leq |\beta| \leq d+1$,

(K3) $\int |\mathbf{x}|^{d+2} \, |\Lambda(|\mathbf{x}|)| d\mathbf{x} < \infty$, and

(K4) $\hat{\Lambda}(\mathbf{s}) \leq \hat{\Lambda}(0)$.

Conditions (K1) through (K3) ensure that the error in the approximation of the Laplacian by the operator Q is $O(\sigma^d)$. For this reason a function that satisfies the conditions above will be referred to as a kernel of order d. Condition (K4) will be used in the stability estimates of Sections 3 and 4.

Due to the radial symmetry of Λ, we have that $\Lambda_\sigma(\mathbf{y}-\mathbf{x}) = \Lambda_\sigma(\mathbf{x}-\mathbf{y})$. In particular, the operator Q acting on Γ can be written as

$$\begin{aligned} Q\Gamma(\mathbf{x}) &= \frac{1}{\sigma^2}\int [\Gamma(\mathbf{y}) - \Gamma(\mathbf{x})]\,\Lambda_\sigma(\mathbf{y}-\mathbf{x})d\mathbf{y} \\ &= \frac{1}{\sigma^2}[(\Lambda_\sigma - \lambda\delta) * \Gamma](\mathbf{x})\,, \end{aligned} \tag{2.4}$$

where δ is a two-dimensional Dirac delta and $\lambda = \int \Lambda(|\mathbf{y}|)d\mathbf{y} = 2\pi\hat{\Lambda}(0)$ is a constant. These facts are the basis for the definition of the numerical methods.

Various ways of discretizing equation (2.1) are possible depending on the way we view the operator Q. The three methods we consider are based on the following discrete versions of the integral operator:

1. PSE method:

$$Q^h\Gamma(\mathbf{x}) = \frac{h^2}{\sigma^2}\sum_{j=1}^{N}\Big[\Gamma(\mathbf{x}^j) - \Gamma(\mathbf{x})\Big]\,\Lambda_\sigma(\mathbf{x}-\mathbf{x}^j)\,. \tag{2.5}$$

2. Method B:

$$Q^h\Gamma(\mathbf{x}) = \frac{h^2}{\sigma^2}\sum_{j=1}^{N}\Gamma(\mathbf{x}^j)\Lambda_\sigma(\mathbf{x}-\mathbf{x}^j) - \frac{\lambda}{\sigma^2}\Gamma(\mathbf{x})\,. \tag{2.6}$$

3. Method C:

$$Q^h\Gamma(\mathbf{x}) = \frac{h^2}{\sigma^2}\sum_{j=1}^{N}\Gamma(\mathbf{x}^j)\,\Big[\Lambda_\sigma(\mathbf{x}-\mathbf{x}^j) - \lambda f_\delta(\mathbf{x}-\mathbf{x}^j)\Big]. \tag{2.7}$$

The PSE method is a direct discretization of equation (2.3), while method B uses the fact that $\lambda = \int \Lambda(|\mathbf{y}|)d\mathbf{y}$ is invariant under translations. Method C uses a cutoff (blob) function f_δ, which approximates the Dirac delta in equation (2.4). We will consider cutoff functions of the form $f_\delta(\mathbf{x}) = \delta^{-2}f(|\mathbf{x}|/\delta)$, where $f \in C^2(\mathbb{R}^2)$ is a radially symmetric function. We say f_δ is a cutoff of order $d+2$ if f satisfies the conditions:

(C1) $\int f(|\mathbf{x}|)d\mathbf{x} = 1$, (C2) $\int \mathbf{x}^\beta f(|\mathbf{x}|)d\mathbf{x} = 0 \quad$ for $1 \leq |\beta| \leq d+1$, and

(C3) $\int |\mathbf{x}|^{d+2} |f(|\mathbf{x}|)|d\mathbf{x} < \infty$.

Note that a cutoff function of order $d+2$ is needed for the operator Q^h in method C to approximate the Laplacian to order d due to the factor of σ^{-2} in Q. This method requires the selection of a kernel Λ of order d and a cutoff f of order $d+2$. The numerical parameters σ and δ will be chosen so that $\sigma = c\delta$ for some fixed positive constant c. The precise choice will be specified in Section 4.

The numerical methods are defined by

$$\frac{d}{dt}\mathbf{x}(\alpha^i, t) = \mathbf{u}(\mathbf{x}(\alpha^i, t), t)\,, \tag{2.8}$$

$$\frac{d}{dt}{\Gamma_h}^i(t) = \nu Q^h {\Gamma_h}^i\,, \tag{2.9}$$

where $\mathbf{x}^i(0) = \mathbf{x}(\alpha^i, 0) = \alpha^i$ for $i = 1, \ldots, N$ are points uniformly distributed on a square lattice of size h in $\mathbb{R}^2$, ${\Gamma_h}^i(0) = \Gamma_0(\alpha^i)$, and $\mathbf{u}(\mathbf{x}, t)$ is the prescribed flow.

3 Convergence of the Continuous Problem

In this section we state and prove results regarding the approximation of the Laplacian by the operator Q and the convergence of solutions of equation (2.1) to solutions of the convection-diffusion equation. Our aim is to establish the results that will be needed in subsequent sections and not to discuss at length the regularity properties of solutions of equation (2.1).

PROPOSITION 3.1 *Assume the function Λ satisfies conditions* (K1) *through* (K3) *outlined in Section* 2. *Then there exists a constant $C > 0$ such that for any function $g \in W^{d+2,p}(\mathbb{R}^2)$ with $1 \leq p \leq \infty$*

$$\|\Delta g - Qg\|_{0,p} \leq C\sigma^d \|g\|_{d+2,p}\,.$$

PROOF: Following [7], in the definition of Qg we expand g in a Taylor series with remainder. Then, for a double index β we have that

$$Qg(\mathbf{x}) = \Delta g(\mathbf{x}) + \frac{d+2}{\sigma^2} \sum_{|\beta|=d+2} \frac{1}{\beta!} \int_0^1 (1-s)^{d+1} \int \partial^\beta g(\mathbf{x} + s\mathbf{z})\mathbf{z}^\beta \Lambda_\sigma(\mathbf{z})d\mathbf{z}\,ds\,.$$

Taking norms and using the triangle inequality, we find that

$$\begin{aligned}&\|(\Delta - Q)g\|_{0,p}\\ &\quad\leq \frac{d+2}{\sigma^2}\ \|g\|_{d+2,p} \sum_{|\beta|=d+2} \frac{C_1}{\beta!} \int_0^1 (1-s)^{d+1} ds \int |\mathbf{z}|^{d+2} |\Lambda_\sigma(\mathbf{z})| d\mathbf{z}\,.\end{aligned}$$

The result follows since

$$\int |\mathbf{z}|^{d+2} |\Lambda_\sigma(\mathbf{z})| d\mathbf{z} = \sigma^{d+2} \int |\mathbf{z}|^{d+2} |\Lambda(|\mathbf{z}|)| d\mathbf{z} = C_2 \sigma^{d+2}\,.$$

∎

COROLLARY 3.2 *Let the assumptions of Proposition* 3.1 *hold. Then there exists a constant* $C > 0$ *such that for any function* $g \in W^{r+d+2,p}(\mathbb{R}^2)$ *with* $0 \leq r$ *and* $1 \leq p \leq \infty$

$$\|\Delta g - Qg\|_{r,p} \leq C\sigma^d \|g\|_{r+d+2,p}\,.$$

PROOF: We make the observation that since $Q\Gamma = 1/\sigma^2(\Lambda_\sigma * \Gamma - \lambda\Gamma)$, one can easily check that $\partial^\beta(Q\Gamma) = Q\partial^\beta\Gamma$ for $|\beta| > 0$. Let β be a double index with $0 \leq |\beta| \leq r$. Then by Proposition 3.1

$$\left\|(\Delta - Q)\partial^\beta g\right\|_{0,p} \leq C_1 \sigma^d \left\|\partial^\beta g\right\|_{d+2,p} \leq C\sigma^d \left\|g\right\|_{r+d+2,p}\,.$$

The result follows. ∎

3.1 Stability of the Integro-Differential Equation

Before stating a stability theorem for equation (2.1), we make the following remark regarding the condition on the Fourier transform of the kernel Λ: Given a function $g \in L^2(\mathbb{R}^2)$, the inequality $\hat{\Lambda}(\mathbf{s}) \leq \hat{\Lambda}(0)$ implies

$$\begin{aligned}2\pi \int \hat{\Lambda}_\sigma(\mathbf{s})\, \hat{g}(\mathbf{s}) \overline{\hat{g}(\mathbf{s})} d\mathbf{s} &\leq 2\pi \hat{\Lambda}(0)\, \|\hat{g}\|_{0,2}^2\\ \iff \int (\widehat{\Lambda_\sigma * g}) \overline{\hat{g}(\mathbf{s})} d\mathbf{s} &\leq \lambda \|g\|_{0,2}^2\\ \iff \int (\Lambda_\sigma * g)(\mathbf{x}) g(\mathbf{x}) d\mathbf{x} &\leq \lambda \|g\|_{0,2}^2\,. \qquad (3.1)\end{aligned}$$

This inequality states that $\int (Qg)(\mathbf{x}) g(\mathbf{x}) \leq 0$, which is key in the following stability theorem:

THEOREM 3.3 *Let Λ satisfy conditions* (K1) *through* (K4) *in Section* 2*. If* $\mathbf{u} \in L^\infty(0,T;W^{r,\infty}(\mathbb{R}^2))$ *and* $\Gamma_0 \in W^{r,2}(\mathbb{R}^2)$*, then equation* (2.1) *has a unique solution in* $L^\infty(0,T;W^{r,2}(\mathbb{R}^2))$*, and there exists a constant* $C = C(\Lambda, \mathbf{u}, T) > 0$ *such that for* $0 < t \le T$

$$\|\Gamma(\cdot,t)\|_{r,2} \le C\|\Gamma_0\|_{r,2}\,. \tag{3.2}$$

PROOF: We provide the proof of existence in order to present a self-contained analysis. For the purposes of this paper, however, the bound in (3.2) is the more relevant result. Let

$$U \in L^\infty(0,T;W^{r,\infty}(\mathbb{R}^2))$$

and

$$F \in L^1(0,T;W^{r,2}(\mathbb{R}^2))\,.$$

Then the equation

$$\frac{\partial \Gamma}{\partial t} + (\mathbf{u}\cdot\nabla)\Gamma + U\Gamma = F\,, \qquad \nabla\cdot\mathbf{u} = 0\,, \tag{3.3}$$

$$\Gamma(\mathbf{x},0) = \Gamma_0(\mathbf{x})\,, \qquad \mathbf{x} \in \mathbb{R}^2\,, \tag{3.4}$$

has a unique solution in $L^\infty(0,T;W^{r,2}(\mathbb{R}^2))$ (see theorem 1.3 in [12]). Multiplying equation (3.3) by Γ and integrating in space, we find that

$$\frac{d}{dt}\|\Gamma\|_{0,2} \le \|U\|_{0,\infty}\|\Gamma\|_{0,2} + \|F(\cdot,t)\|_{0,2}\,,$$

and by Gronwall's inequality we conclude that

$$\|\Gamma(\cdot,t)\|_{0,2} \le \gamma_1\left[\|\Gamma_0\|_{0,2} + \int_0^t \|F(\cdot,s)\|_{0,2}\,ds\right], \tag{3.5}$$

where γ_1 depends on $\|U\|_{0,\infty}$ and T. Consider $F = Qf$ for some $f \in L^2(\mathbb{R}^2)$. Since $Qf = (1/\sigma^2)(\Lambda_\sigma * f - \lambda f)$, it is clear that $\|Qf\|_{0,2} \le C_\sigma\|f\|_{0,2}$ for $C_\sigma = (\|\Lambda\|_{0,1} + \lambda)/\sigma^2$. Let Φ be the mapping defined by $\Gamma = \Phi f$ where Γ satisfies the equation

$$\frac{\partial \Gamma}{\partial t} + (\mathbf{u}\cdot\nabla)\Gamma + U\Gamma = \nu Qf\,, \qquad \nabla\cdot\mathbf{u} = 0\,, \tag{3.6}$$

$$\Gamma(\mathbf{x},0) = \Gamma_0(\mathbf{x})\,, \qquad \mathbf{x} \in \mathbb{R}^2\,. \tag{3.7}$$

Then, using (3.5), we have that for $f_1, f_2 \in L^\infty(0,T;L^2(\mathbb{R}^2))$

$$\|\Phi f_1 - \Phi f_2\|_{0,2} \le \gamma_1 C_\sigma \int_0^t \|f_1 - f_2\|_{0,2}\,.$$

We now choose a final time T^* such that $\gamma_1 C_\sigma T^* \le \alpha < 1$. Thus,

$$\operatorname*{ess\,sup}_{0\le t\le T^*} \|\Phi f_1 - \Phi f_2\|_{0,2} \le \alpha \operatorname*{ess\,sup}_{0\le t\le T^*} \|f_1 - f_2\|_{0,2}\,.$$

Therefore Φ is a contraction, and it has a unique fixed point Γ^* in the space $L^\infty(0,T^*;L^2(\mathbb{R}^2))$, which is the solution of equation (3.6). This argument can be repeated for the intervals $[T^*, 2T^*]$, $[2T^*,\ 3T^*]$, and so on, so that the solution is valid to time T.

In order to establish existence in the space $L^\infty(0,T;W^{r,2}(\mathbb{R}^2))$, we differentiate equation (3.6) and use the fact that $\partial^\beta(Q\Gamma) = Q\partial^\beta\Gamma$ to find that $\partial^\beta\Gamma$ satisfies equation (3.6) with a right-hand side term that contains derivatives of Γ of order lower than β and derivatives of $\mathbf{u}$ and U. The same arguments as above yield existence and uniqueness of the solution of equation (3.6) in $L^\infty(0,T;W^{r,2}(\mathbb{R}^2))$.

To obtain the bound independent of ν and σ, we multiply equation (2.1) by $\Gamma(\mathbf{x})$ and integrate over $\mathbf{x}$ to obtain

$$\begin{aligned}\frac{d}{dt}\int |\Gamma(\mathbf{x})|^2 d\mathbf{x} &= 2\nu \int (Q\Gamma)(\mathbf{x})\Gamma(\mathbf{x})d\mathbf{x}\\ &= \frac{2\nu}{\sigma^2}\int (\Lambda_\sigma * \Gamma)(\mathbf{x})\Gamma(\mathbf{x}) - \lambda|\Gamma(\mathbf{x})|^2\, d\mathbf{x} \le 0\,,\end{aligned}$$

where the last inequality follows in view of (3.1). Hence, we have

$$\|\Gamma(\cdot,t)\|_{0,2} \le \|\Gamma_0\|_{0,2}\,. \tag{3.8}$$

In order to bound $\|\partial^\beta\Gamma\|_{0,2}$ for a double index with $|\beta| = 1$, we proceed as follows. First, recall that $\partial^\beta(Q\Gamma) = Q\partial^\beta\Gamma$. Second, we differentiate equation (2.1) to get

$$\frac{\partial(\partial^\beta\Gamma)}{\partial t} + (\mathbf{u}\cdot\nabla)(\partial^\beta\Gamma) = \nu Q\partial^\beta\Gamma - \partial^\beta\mathbf{u}\cdot\nabla\Gamma\,.$$

Proceeding as above, we have that

$$\frac{d}{dt}\|\nabla\Gamma\|_{0,2} \le \gamma\|\nabla\Gamma\|_{0,2}\,,$$

where γ depends on $\|\mathbf{u}\|_{|\beta|,\infty}$. By Gronwall's inequality coupled with expression (3.8), we get

$$\|\Gamma(\cdot,t)\|_{1,2} \leq C\|\Gamma_0\|_{1,2}\,.$$

For $2 \leq |\beta| \leq r$, the equation for $\partial^\beta \Gamma$ is equation (3.6) with a right-hand side that contains derivatives of Γ of order lower than β. Expression (3.2) follows by induction. ∎

3.2 Convergence Result for the Continuous Problem

The results in the previous sections imply the convergence of the solutions of equation (2.1) to solutions of equation (1.1). We first state a classical result regarding solutions of equation (1.1) and then present the convergence result for the continuous problem. In Section 4 we discuss the convergence of the numerical solution to the solution of equation (2.1).

PROPOSITION 3.4 *Let* $\mathbf{u} \in L^\infty(0,T;W^{r,\infty}(\mathbb{R}^2))$ *and* $\Gamma_0 \in W^{r,2}(\mathbb{R}^2)$. *Then equation* (1.1) *has a unique solution in* $L^\infty(0,T;W^{r,2}(\mathbb{R}^2))$, *and there exists a constant* $C = C(\mathbf{u},T) > 0$ *such that for* $0 < t \leq T$

$$\|\Gamma(\cdot,t)\|_{r,2} \leq C\|\Gamma_0\|_{r,2}\,. \tag{3.9}$$

THEOREM 3.5 *Assume that* $\mathbf{u} \in L^\infty(0,T;W^{r,\infty}(\mathbb{R}^2))$, *and let* Λ *satisfy the conditions of Theorem* 3.3. *Let* Γ *and* Γ^σ *be the solutions of equation* (1.1) *and equation* (2.1), *respectively. Then there is a constant* $C = C(\mathbf{u},\Lambda,T) > 0$ *such that for* $\Gamma_0 \in W^{r+d+2,2}(\mathbb{R}^2)$ *and for* $0 \leq t \leq T$

$$\|\Gamma - \Gamma^\sigma\|_{r,2} \leq C\nu\sigma^d\|\Gamma_0\|_{r+d+2,2}\,. \tag{3.10}$$

PROOF: Set $g = \Gamma - \Gamma^\sigma$. Then we have

$$\frac{\partial g}{\partial t} + (\mathbf{u}\cdot\nabla)g - \nu Q g = \nu(\Delta - Q)\Gamma\,, \quad g(\cdot,0) = 0\,.$$

From the result of Theorem 3.3, we have that

$$\|g(\cdot,t)\|_{r,2} \leq C_1\nu\int_0^t \|(\Delta - Q)\Gamma\|_{r,2}d\tau\,.$$

By Corollary 3.2 and Proposition 3.4, we have that

$$\|g(\cdot,t)\|_{r,2} \leq C\nu\sigma^d\|\Gamma_0\|_{r+d+2,2}\,.$$

∎

4 Convergence of the Particle Methods

We have established the convergence of the solution Γ^σ of equation (2.1) to the solution Γ of the convection-diffusion equation. In this section we discuss the consistency and stability of the three numerical methods defined in Section 2. The convergence proofs for methods B and C require additional conditions on the numerical parameters. These conditions will be discussed as they are introduced.

We will make use of the following result found in [12, p. 262]. We present it as a lemma and omit the proof.

LEMMA 4.1 *Let $g \in W^{k,1}(\mathbb{R}^2)$ with $k \geq 3$ and let α^j be uniformly distributed points in $\mathbb{R}^2$. Then*

$$\left| \int g(\alpha) d\alpha - \sum_{j=1}^{N} g(\alpha^j) h^2 \right| \leq C h^k \|g\|_{k,1} \,. \tag{4.1}$$

4.1 PSE Method

Recall that for the PSE method the discrete integral operator is given by

$$Q^h \Gamma(\mathbf{x}) = \frac{h^2}{\sigma^2} \sum_{j=1}^{N} \left[\Gamma(\mathbf{x}^j) - \Gamma(\mathbf{x}) \right] \Lambda_\sigma(\mathbf{x} - \mathbf{x}^j) \,.$$

THEOREM 4.2 *Let $\Gamma_0 \in W^{m+r,2}(\mathbb{R}^2)$ and $\mathbf{u} \in L^\infty(0, T; W^{m+r,\infty}(\mathbb{R}^2))$ where $0 \leq r$. Let Λ_σ satisfy conditions* (K1) *through* (K4) *with $4 \leq d+2 \leq m$. Let Γ be the solution of equation* (2.1). *Let $\mathbf{x}^j(0)$, $j = 1, \ldots, N$, be points on a uniform square grid of size h in $\mathbb{R}^2$, and let $\mathbf{x}^j(t)$ evolve according to equation* (2.8). *Then there exists a constant C such that for $\sigma \leq 1$,*

$$\left\| Q\Gamma - \frac{h^2}{\sigma^2} \sum_{j=1}^{N} \left[\Gamma(\mathbf{x}^j) - \Gamma(\mathbf{x}) \right] \Lambda_\sigma(\mathbf{x} - \mathbf{x}^j) \right\|_{r,2} \leq C \, \|\Gamma_0\|_{m+r,2} \left(\frac{h^m}{\sigma^{m+r+2}} \right)$$

PROOF: Define the discretization error $e(\mathbf{x})$ as

$$e(\mathbf{x}) = Q\Gamma(\mathbf{x}) - \frac{h^2}{\sigma^2} \sum_{j=1}^{N} \left[\Gamma(\mathbf{x}^j) - \Gamma(\mathbf{x}) \right] \Lambda_\sigma(\mathbf{x} - \mathbf{x}^j) \,. \tag{4.2}$$

In order to bound the norm of $e(\mathbf{x})$ we use Lemma 4.1 with $k = m$ and the function $g(\alpha) = \frac{1}{\sigma^2} \left[\Gamma(\mathbf{y}(\alpha, t)) - \Gamma(\mathbf{x}) \right] \Lambda_\sigma(\mathbf{x} - \mathbf{y}(\alpha, t))$. Then we have that

$$|e(\mathbf{x})| \leq \frac{Ch^m}{\sigma^2}\left[\sum_{0\leq|\beta|+|\theta|\leq m}\int\left|\partial_\alpha^\theta\Lambda_\sigma(\mathbf{x}-\mathbf{y}(\alpha,t))\partial_\alpha^\beta\Gamma(\mathbf{y}(\alpha,t))\right|d\alpha\right] + \frac{Ch^m}{\sigma^2}|\Gamma(\mathbf{x})|\,\|\Lambda_\sigma\|_{m,1}$$

and by the triangle inequality and properties of convolutions, we get that

$$\|e\|_{0,2} \leq \frac{Ch^m}{\sigma^2}\sum_{0\leq|\beta|+|\theta|\leq m}\sqrt{\int d\mathbf{x}\left[\int\left|\partial_\alpha^\theta\Lambda_\sigma(\mathbf{y}(\alpha,t))\partial_\alpha^\beta\Gamma(\mathbf{x}-\mathbf{y}(\alpha,t))\right|d\alpha\right]^2} + \frac{Ch^m}{\sigma^2}\|\Gamma\|_{0,2}\,\|\Lambda_\sigma\|_{m,1}.$$

By Minkowski's inequality,

$$\|e\|_{0,2} \leq \frac{Ch^m}{\sigma^2}\sum_{0\leq|\beta|+|\theta|\leq m}\int d\alpha\sqrt{\int\left|\partial_\alpha^\theta\Lambda_\sigma(\mathbf{y}(\alpha,t))\partial_\alpha^\beta\Gamma(\mathbf{x}-\mathbf{y}(\alpha,t))\right|^2 d\mathbf{x}} + \frac{Ch^m}{\sigma^2}\|\Gamma\|_{0,2}\,\|\Lambda_\sigma\|_{m,1}\,.$$

By repeated application of the chain rule, derivatives of $g(\alpha)$ up to order m are sums of derivatives with respect to $\mathbf{y}$ of $\Lambda_\sigma(\mathbf{x}-\mathbf{y})\Gamma(\mathbf{y})$ multiplied by derivatives of $\mathbf{y}(\alpha,t)$ with respect to α. The latter are assumed to be bounded. Therefore, there are constants independent of $\mathbf{y}$ and t such that

$$\|e\|_{0,2} \leq \frac{Ch^m}{\sigma^2}\|\Lambda_\sigma\|_{m,1}\,\|\Gamma\|_{m,2} \leq \frac{Ch^m}{\sigma^{m+2}}\,\|\Gamma\|_{m,2}\,,$$

where the last inequality follows from $\|\Lambda_\sigma\|_{m,1} \leq C\sigma^{-m}$.

In order to bound $\|e\|_{r,2}$, we must bound the L^2-norms of derivatives of $e(\mathbf{x})$. Applying (4.1) to the function $g(\alpha) = \partial_\alpha^\beta\frac{1}{\sigma^2}\{[\Gamma(\mathbf{y}(\alpha,t))-\Gamma(\mathbf{x})]\Lambda_\sigma(\mathbf{x}-\mathbf{y}(\alpha,t))\}$, we find that for $|\beta|\leq r$,

$$\left\|\partial^\beta e\right\|_{0,2} \leq \frac{Ch^m}{\sigma^2}\|\Lambda_\sigma\|_{|\beta|+m,1}\,\|\Gamma\|_{|\beta|+m,2} \leq \frac{Ch^m}{\sigma^{|\beta|+m+2}}\,\|\Gamma\|_{|\beta|+m,2} \leq \frac{Ch^m}{\sigma^{r+m+2}}\,\|\Gamma\|_{r+m,2}$$

for $\sigma\leq 1$. Then,

$$\|e\|_{r,2} \leq \frac{Ch^m}{\sigma^{r+m+2}}\,\|\Gamma\|_{m+r,2}\,. \tag{4.3}$$

The proof is completed by combining (4.3) and Theorem 3.3. ∎

We are now ready to state and prove a convergence theorem for the PSE method.

THEOREM 4.3 (Convergence of PSE Method) *Let* $\mathbf{x}^i(0) = \alpha^i$ *be points distributed uniformly in* $\mathbb{R}^2$, *and assume that* $\mathbf{u} \in L^\infty(0,T;W^{m+3,\infty}(\mathbb{R}^2))$ *and* $\Gamma_0 \in W^{m+3,2}(\mathbb{R}^2)$ *with* $4 \le d+2 \le m$. *Assume that* Λ *satisfies conditions* (K1) *through* (K4). *Denote by* ${\Gamma_h}^i(t)$ *and* $\Gamma^i(t)$ *the respective solutions of the equations*

$$\frac{d{\Gamma_h}^i}{dt} = \frac{\nu h^2}{\sigma^2}\sum_{j=1}^{N}\left[{\Gamma_h}^j - {\Gamma_h}^i\right]\Lambda_\sigma(\mathbf{x}^j - \mathbf{x}^i) \quad \textit{and} \quad \frac{d\Gamma^i}{dt} = \nu\Delta\Gamma(\mathbf{x}^i)$$

where $d\mathbf{x}^i/dt = \mathbf{u}(\mathbf{x}^i)$. *Then there is a constant* K *such that*

$$\|\Gamma_h - \Gamma\|_{0,2,h} \le K\nu\|\Gamma_0\|_{m+3,2}\left(\sigma^d + \frac{h^m}{\sigma^{m+2}} + \frac{h^{m+3/2}}{\sigma^{m+5}}\right). \tag{4.4}$$

PROOF: Define $e_k(t) = {\Gamma_h}^k - \Gamma^k$; then

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\sum_k h^2 e_k^2 &= \nu\sum_k h^2 e_k\left[Q^h{\Gamma_h}^k - \Delta\Gamma(\mathbf{x}^k)\right]\\ &= \nu\sum_k h^2 e_k\left[(Q^h{\Gamma_h}^k - Q^h\Gamma^k) + (Q^h\Gamma^k - \Delta\Gamma^k)\right]\\ &= \nu(T_1 + T_2)\,,\end{aligned} \tag{4.5}$$

where Q^h is defined in equation (2.5). Consider T_1.

$$\begin{aligned}T_1 &= \sum_k h^2 e_k Q^h e_k\\ &= \frac{1}{\sigma^2}\sum_k h^2 e_k \sum_j h^2 e_j \Lambda_\sigma(\mathbf{x}^k - \mathbf{x}^j) - \frac{1}{\sigma^2}\sum_k h^2 e_k^2 \sum_j h^2 \Lambda_\sigma(\mathbf{x}^k - \mathbf{x}^j)\,.\end{aligned}$$

We use the algebraic inequality $2e_ke_j \le e_k^2 + e_j^2$ to write

$$\begin{aligned}T_1 &\le \frac{1}{2\sigma^2}\sum_k h^2\sum_j h^2(e_j^2 + e_k^2)\Lambda_\sigma(\mathbf{x}^k - \mathbf{x}^j)\\ &\quad - \frac{1}{\sigma^2}\sum_k h^2 e_k^2\sum_j h^2\Lambda_\sigma(\mathbf{x}^k - \mathbf{x}^j)\\ &= \frac{1}{\sigma^2}\sum_k h^2 e_k^2\sum_j h^2\Lambda_\sigma(\mathbf{x}^k - \mathbf{x}^j)\\ &\quad - \frac{1}{\sigma^2}\sum_k h^2 e_k^2\sum_j h^2\Lambda_\sigma(\mathbf{x}^k - \mathbf{x}^j) = 0\end{aligned} \tag{4.6}$$

due to the symmetry of Λ_σ.

Consider now the second term in equation (4.5). Hölder's inequality implies that

$$\left|\sum_k h^2 e_k \left[Q^h\Gamma\left(\mathbf{x}^k\right) - \Delta\Gamma\left(\mathbf{x}^k\right)\right]\right| \le \|\Gamma_h - \Gamma\|_{0,2,h}\ \|(Q^h - \Delta)\Gamma\|_{0,2,h}\,. \tag{4.7}$$

We now make use of Lemma 4.1 with $k = 3$ and the function g^2 where $g(\alpha) = Q^h\Gamma(\mathbf{x}(\alpha,t)) - \Delta\Gamma(\mathbf{x}(\alpha,t))$. Then

$$\begin{aligned}\|g\|_{0,2,h}^2 = \sum_\ell h^2 g^2(\alpha^\ell) &\le \|g\|_{0,2}^2 + Ch^3\|g^2\|_{3,1}\\ &\le \|g\|_{0,2}^2 + Ch^3\|g\|_{3,2}^2\,.\end{aligned}$$

The algebraic inequality $a^2 + b^2 \le (|a| + |b|)^2$ implies that

$$\|g\|_{0,2,h} \le \|g\|_{0,2} + Ch^{3/2}\|g\|_{3,2}\,.$$

The norms in the last expression contain integrals with respect to α. These can be viewed as integrals with respect to $\mathbf{x}$ multiplied by a constant that depends on the transformation $\alpha \to \mathbf{x}(\alpha,t)$.

Combining the results of Proposition 3.1, Theorem 3.3, and Theorem 4.2, once with $r = 0$ and once more with $r = 3$, we find that

$$\|g\|_{0,2} \le C_1\|\Gamma_0\|_{m,2}\left(\sigma^d + \frac{h^m}{\sigma^{m+2}}\right)$$

and

$$\|g\|_{3,2} \le C_2\|\Gamma_0\|_{m+3,2}\left(\sigma^d + \frac{h^m}{\sigma^{m+5}}\right).$$

This yields

$$\begin{aligned}\|g\|_{0,2,h} &\le C\|\Gamma_0\|_{m+3,2}\left[\sigma^d\left(C_1 + h^{3/2}C_2\right) + \frac{h^m}{\sigma^{m+2}}C_3 + \frac{h^{m+3/2}}{\sigma^{m+5}}C_4\right]\\ &\le C\|\Gamma_0\|_{m+3,2}\left(\sigma^d + \frac{h^m}{\sigma^{m+2}} + \frac{h^{m+3/2}}{\sigma^{m+5}}\right).\end{aligned} \tag{4.8}$$

Equation (4.5) can be rewritten using (4.6) and (4.8) to get

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\|\Gamma_h - \Gamma\|_{0,2,h}^2 &= \frac{1}{2}\frac{d}{dt}\sum_k h^2 e_k^2\\ &= \nu(T_1 + T_2)\\ &\le C\nu\|\Gamma_h - \Gamma\|_{0,2,h}\ \|\Gamma_0\|_{m+3,2}\left(\sigma^d + \frac{h^m}{\sigma^{m+2}} + \frac{h^{m+3/2}}{\sigma^{m+5}}\right).\end{aligned}$$

Therefore, we have that

$$\frac{d}{dt}\|\Gamma_h - \Gamma\|_{0,2,h} \le C\nu \, \|\Gamma_0\|_{m+3,2} \left(\sigma^d + \frac{h^m}{\sigma^{m+2}} + \frac{h^{m+3/2}}{\sigma^{m+5}} \right),$$

which implies the desired result. Note that K in (4.4) does not depend on ν, σ, or h. ∎

We remark that since $4 \le d+2 \le m$ by assumption, one can choose a relation of the type $\sigma = Ch^q$ for some exponent $0 < q < (m + \frac{3}{2})/(m+5)$. We make the observation that the errors in (4.4) are of the same order when $q = \frac{1}{2}$ and $m = d+2$.

4.2 Method B

We state the corresponding theorems for method B. In the remaining sections the proofs of the theorems will only be sketched since they are very similar to the proof already presented. The discrete operator of method B is given by

$$Q^h\Gamma(\mathbf{x}) = \frac{h^2}{\sigma^2} \sum_{j=1}^{N} \Gamma(\mathbf{x}^j)\Lambda_\sigma(\mathbf{x} - \mathbf{x}^j) - \frac{\lambda}{\sigma^2}\Gamma(\mathbf{x})\,.$$

Notice that this differs from the PSE method only in the way the last term is discretized.

THEOREM 4.4 *Let* $\mathbf{u} \in L^\infty(0,T; W^{m+r,\infty}(\mathbb{R}^2))$ *and* $\Gamma_0 \in W^{m+r,2}(\mathbb{R}^2)$, *where* $0 \le r$. *Let* Λ_σ *satisfy conditions* (K1) *through* (K4) *with* $4 \le d+2 \le m$. *Let* Γ *be the solution of equation* (2.1). *Let* $\mathbf{x}^j(0)$, $j = 1, \ldots, N$, *be points on a uniform square grid of size* h *in* $\mathbb{R}^2$ *and let* $\mathbf{x}^j(t)$ *evolve according to equation* (2.8). *Then there exists a constant* C *such that for* $\sigma \le 1$,

$$\left\| Q\Gamma - \left[\frac{h^2}{\sigma^2} \sum_{j=1}^{N} \Gamma(\mathbf{x}^j)\Lambda_\sigma(\cdot - \mathbf{x}^j) - \frac{\lambda}{\sigma^2}\Gamma(\cdot) \right] \right\|_{r,2} \le C\,\|\Gamma_0\|_{m+r,2} \left(\frac{h^m}{\sigma^{m+r+2}} \right).$$

PROOF: Define the discretization error as

$$\begin{aligned} e(\mathbf{x}) &= Q\Gamma(\mathbf{x}) - \left[\frac{h^2}{\sigma^2} \sum_{j=1}^{N} \Gamma(\mathbf{x}^j)\Lambda_\sigma(\mathbf{x} - \mathbf{x}^j) - \frac{\lambda}{\sigma^2}\Gamma(\mathbf{x}) \right] \\ &= \frac{1}{\sigma^2} \left[\int \Gamma(\mathbf{y})\Lambda_\sigma(\mathbf{x} - \mathbf{y})d\mathbf{y} - h^2 \sum_{j=1}^{N} \Gamma(\mathbf{x}^j)\Lambda_\sigma(\mathbf{x} - \mathbf{x}^j) \right] \end{aligned}$$

since $\lambda = \int \Lambda_\sigma(\mathbf{x} - \mathbf{y})d\mathbf{y}$. The bound for $\|e\|_{r,2}$ is obtained in exactly the same way as in Theorem 4.2. The result follows. ∎

The convergence proof of method B requires the condition

$$\nu\left(\frac{h^m}{\sigma^{m+2}}\right)\le C_v \tag{4.9}$$

where C_v is any positive constant and m is determined by the smoothness of the flow. For simplicity we set $C_v = 1$ for the rest of the paper. The reason for this condition appears to be technical, and its necessity will become clear in the proof.

We recall that in [7] the authors required the condition

$$\nu \le C_s\sigma^2$$

for a fixed constant C_s. Two important distinctions between these conditions should be made. First, the condition in [7] was needed to prove stability of the integro-differential equation (2.1) while in the present paper no such condition is needed to prove stability of the continuous problem. Second, the condition in [7] is an impediment to convergence of the PSE method because the limit of vanishing numerical parameters cannot be reached while maintaining the condition. The requirement (4.9) can be maintained for any fixed constant C_v by choosing σ and h appropriately as they are decreased to zero. For instance, the choice $\sigma = Ch^q$ for $q < m/(m+2)$ allows condition (4.9) to be satisfied for h small enough.

THEOREM 4.5 (Convergence of Method B) *Let $\mathbf{x}^i(0)=\alpha^i$ be uniformly distributed points in $\mathbb{R}^2$, and assume that $\mathbf{u}\in L^\infty(0,T;W^{m+3,\infty}(\mathbb{R}^2))$ and $\Gamma_0\in W^{m+3,2}(\mathbb{R}^2)$ with $4\le d+2\le m$. Assume that Λ satisfies conditions* (K1) *through* (K4) *and that the condition* (4.9) *is satisfied for $C_v=1$. Denote by ${\Gamma_h}^i(t)$ and $\Gamma^i(t)$ the respective solutions of the equations*

$$\frac{d{\Gamma_h}^i}{dt}=\frac{\nu h^2}{\sigma^2}\sum_{j=1}^{N}[{\Gamma_h}^j-{\Gamma_h}^i]\Lambda_\sigma(\mathbf{x}^j-\mathbf{x}^i)\quad \textit{and}\quad \frac{d\Gamma^i}{dt}=\nu\Delta\Gamma(\mathbf{x}^i)\,,$$

where $d\mathbf{x}^i/dt=\mathbf{u}(\mathbf{x}^i)$. Then there is a constant K such that

$$\|\Gamma_h-\Gamma\|_{0,2,h}\le K\nu\|\Gamma_0\|_{m+3,2}\left(\sigma^d+\frac{h^m}{\sigma^{m+2}}+\frac{h^{m+3/2}}{\sigma^{m+5}}\right). \tag{4.10}$$

PROOF: We only sketch the proof. Define $e_k(t)={\Gamma_h}^k-\Gamma^k$, then

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\sum_k h^2e_k^2 &= \nu\sum_k h^2e_k\left[Q^h{\Gamma_h}^k-\Delta\Gamma(\mathbf{x}^k)\right]\\ &=\nu\sum_k h^2e_k\left[(Q^h{\Gamma_h}^k-Q^h\Gamma^k)+(Q^h\Gamma^k-\Delta\Gamma^k)\right]\\ &=\nu(T_1+T_2)\,,\end{aligned}\tag{4.11}$$

where Q^h is defined in equation (2.6).

T_1 is now given by

$$T_1 = \sum_k h^2 e_k Q^h e_k = \frac{1}{\sigma^2} \sum_k h^2 e_k \sum_j h^2 e_j \Lambda_\sigma(\mathbf{x}^k - \mathbf{x}^j) - \frac{\lambda}{\sigma^2} \sum_k h^2 e_k^2 \,.$$

Proceeding as in the proof of Theorem 4.3, we find that

$$T_1 \leq \frac{1}{\sigma^2} \sum_k h^2 e_k^2 \left[\sum_j h^2 \Lambda_\sigma(\mathbf{x}^k - \mathbf{x}^j) - \lambda \right],$$

where the factor in brackets can be estimated using Lemma 4.1 once again. This yields

$$\sum_j h^2 \Lambda_\sigma(\mathbf{x}^k - \mathbf{x}^j) - \lambda \leq C \frac{h^m}{\sigma^m}\,,$$

which in turn implies that

$$\nu T_1 \leq C \|\Gamma_h - \Gamma\|_{0,2,h}^2 \, \frac{\nu h^m}{\sigma^{m+2}} \leq C \|\Gamma_h - \Gamma\|_{0,2,h}^2 \tag{4.12}$$

from condition (4.9).

T_2 is bounded in the same way as in Theorem 4.3 so that

$$\begin{aligned} &\frac{d}{dt} \|\Gamma_h - \Gamma\|_{0,2,h} \\ &\quad \leq C \|\Gamma_h - \Gamma\|_{0,2,h} + C\nu \|\Gamma_0\|_{m+3,2} \left(\sigma^d + \frac{h^m}{\sigma^{m+2}} + \frac{h^{m+3/2}}{\sigma^{m+5}} \right). \end{aligned} \tag{4.13}$$

Gronwall's lemma implies the desired result. ∎

4.3 Method C

The third method is one in which an approximation of the Dirac delta by a cutoff function has been introduced. The discrete operator is given by

$$Q^h \Gamma(\mathbf{x}) = \frac{h^2}{\sigma^2} \sum_{j=1}^{N} \Gamma(\mathbf{x}^j) \left[\Lambda_\sigma(\mathbf{x} - \mathbf{x}^j) - \lambda f_\delta(\mathbf{x} - \mathbf{x}^j) \right],$$

where the numerical parameters satisfy the conditions of Section 2.

THEOREM 4.6 *Let Λ_σ satisfy conditions* (K1) *through* (K4)*, and let f_δ satisfy conditions* (C1) *through* (C3) *in Section* 2 *with $\sigma = c\delta$ for a fixed constant c. Let $\mathbf{u} \in L^\infty(0,T;W^{m+r,\infty}(\mathbb{R}^2))$ and $\Gamma_0 \in W^{m+r,2}(\mathbb{R}^2)$, where $4 \le d+2 \le m$ and $0 \le r$. Let Γ be the solution of equation* (2.1)*. Let $\mathbf{x}^j(0)$, $j = 1,\dots,N$, be points on a uniform square grid of size h in $\mathbb{R}^2$, and let $\mathbf{x}^j(t)$ evolve according to equation* (2.8)*. Then there exists a constant C such that for $\sigma \le 1$,*

$$\left\| Q\Gamma - \frac{h^2}{\sigma^2}\sum_{j=1}^N \Gamma(\mathbf{x}^j)\left[\Lambda_\sigma(\mathbf{x}-\mathbf{x}^j) - \lambda f_\delta(\mathbf{x}-\mathbf{x}^j)\right]\right\|_{r,2} \le C\|\Gamma_0\|_{m+r,2}\left(\sigma^d + \frac{h^m}{\sigma^{m+r+2}}\right)$$

PROOF: Define the discretization error as $e(\mathbf{x}) = e_1(\mathbf{x}) + e_2(\mathbf{x}) + e_3(\mathbf{x})$, where

$$\begin{aligned} e_1(\mathbf{x}) &= \frac{1}{\sigma^2}\left[\int \Gamma(\mathbf{y})\Lambda_\sigma(\mathbf{x}-\mathbf{y})d\mathbf{y} - h^2\sum_{j=1}^N \Gamma(\mathbf{x}^j)\Lambda_\sigma(\mathbf{x}-\mathbf{x}^j)\right] \\ e_2(\mathbf{x}) &= -\frac{\lambda}{\sigma^2}\left[\Gamma(\mathbf{x}) - \int \Gamma(\mathbf{y})f_\delta(\mathbf{x}-\mathbf{y})d\mathbf{y}\right] \\ e_3(\mathbf{x}) &= -\frac{\lambda}{\sigma^2}\left[\int \Gamma(\mathbf{y})f_\delta(\mathbf{x}-\mathbf{y})d\mathbf{y} - h^2\sum_{j=1}^N \Gamma(\mathbf{x}^j)f_\delta(\mathbf{x}-\mathbf{x}^j)\right]. \end{aligned}$$

The bounds for $\|e_1\|_{r,2}$ and $\|e_3\|_{r,2}$ are found using Lemma 4.1 as in the proof of Theorem 4.5. The results are

$$\|e_1\|_{r,2} \le \frac{Ch^m}{\sigma^2}\|\Lambda_\sigma\|_{r+m,1}\ \|\Gamma\|_{r+m,2} \le \frac{Ch^m}{\sigma^{r+m+2}}\ \|\Gamma\|_{r+m,2} \tag{4.14}$$

$$\|e_3\|_{r,2} \le \frac{Ch^m}{\sigma^2}\|f_\delta\|_{r+m,1}\ \|\Gamma\|_{r+m,2} \le \frac{Ch^m}{\sigma^{r+m+2}}\ \|\Gamma\|_{r+m,2} \tag{4.15}$$

where the last inequality follows from $\|f_\delta\|_{m,1} \le C\delta^{-m}$ and $\sigma = c\delta$.

The remaining term can be written as $e_2(\mathbf{x}) = (\lambda/\sigma^2)[(\Gamma * f_\delta)(\mathbf{x}) - \Gamma(\mathbf{x})]$. The bound for $\|e_2\|$ can be estimated in a way analogous to the proof of Proposition 3.1; the details are found in [12, p. 267]. The result is

$$\|e_2\|_{0,2} \le \frac{C\delta^{d+2}}{\sigma^2}\|\Gamma\|_{d,2} \le C'\sigma^d\|\Gamma\|_{d,2}$$

since $\sigma = c\delta$. In the same way we get that

$$\|e_2\|_{r,2} \le C\sigma^d\|\Gamma\|_{d+r,2}. \le C\sigma^d\|\Gamma\|_{m+r,2}. \tag{4.16}$$

The proof is completed by combining (4.14) through (4.16) and Theorem 3.3. ∎

So far in the analysis of method C, the kernel Λ_σ and the cutoff f_δ have been required to satisfy the conditions specified in Section 2. We now add one more condition that relates the two functions. It is used to establish the discrete version of inequality (3.1). Let the Fourier transforms of Λ and f be such that for some positive constant c we have that

$$\hat{\Lambda}(c|\mathbf{s}|) \leq \lambda \hat{f}(|\mathbf{s}|) \tag{4.17}$$

for all $\mathbf{s} \in \mathbb{R}^2$. We remark that $\hat{\Lambda}$ and $\hat{f}$ are radially symmetric functions.

While different conditions may be devised to replace (4.17), it is natural to expect the need for a condition that connects the kernel Λ_σ and the cutoff f_δ. Since $\lambda = 2\pi\hat{\Lambda}(0)$ and $2\pi\hat{f}(0) = 1$ from (C1), then (4.17) is equivalent to $\hat{f}(0)\hat{\Lambda}(c\mathbf{s}) \leq \hat{\Lambda}(0)\hat{f}(\mathbf{s})$. For $c = 1$, the condition says that the normalized Fourier transform of Λ must be no greater than the normalized transform of f. The constant c has been included to provide more generality.

A heuristic argument that indicates that condition (4.17) can be satisfied is the following. Based on conditions (K1) through (K3) and (C1) through (C3) in Section 2, the Fourier transforms of Λ and f satisfy for $s = |\mathbf{s}|$

$$\hat{\Lambda}(s) = \hat{\Lambda}(0) - s^2 + O(s^{d+2}) \quad \text{and} \quad \lambda\hat{f}(s) = \hat{\Lambda}(0) + O(s^{d+2}),$$

so condition (4.17) is satisfied for small s since $\hat{\Lambda}$ is concave down while $\hat{f}$ is *flatter* near the origin. To maintain this relation for large values of s, the constant c must be chosen so that $\hat{f}$ decays no faster than $\hat{\Lambda}$ as $|\mathbf{s}| \to \infty$. Examples of these functions are given in the last section.

THEOREM 4.7 (Convergence of Method C) *Let $\mathbf{x}^i(0) = \alpha^i$ be uniformly distributed points in $\mathbb{R}^2$ and assume that $\mathbf{u} \in L^\infty(0,T;W^{m+3,\infty}(\mathbb{R}^2))$ and $\Gamma_0 \in W^{m+3,2}(\mathbb{R}^2)$ with $4 \leq d+2 \leq m$. Assume that Λ satisfies conditions* (K1) *through* (K4) *and f satisfies conditions* (C1) *through* (C3) *in Section* 2. *Assume also that Λ and f satisfy inequality* (4.17) *for some constant c and let $\sigma = c\delta$. Denote by ${\Gamma_h}^i(t)$ and $\Gamma^i(t)$ the respective solutions of the equations*

$$\frac{d{\Gamma_h}^i}{dt} = \frac{\nu h^2}{\sigma^2}\sum_{j=1}^{N}{\Gamma_h}^j[\Lambda_\sigma(\mathbf{x}^i - \mathbf{x}^j) - \lambda f_\delta(\mathbf{x}^i - \mathbf{x}^j)],$$
$$\frac{d\Gamma^i}{dt} = \nu\Delta\Gamma(\mathbf{x}^i),$$

where $d\mathbf{x}^i/dt = \mathbf{u}(\mathbf{x}^i)$. *Then there is a constant* K *such that*

$$\|\Gamma_h - \Gamma\|_{0,2,h} \le K\,\nu\,\|\Gamma_0\|_{m+3,2}\left(\sigma^d + \frac{h^m}{\sigma^{m+2}} + \frac{h^{m+3/2}}{\sigma^{m+5}}\right). \tag{4.18}$$

PROOF: Define $e_k(t) = {\Gamma_h}^k - \Gamma^k$; then

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\sum_k h^2 e_k^2 &= \nu\sum_k h^2 e_k\left[Q^h{\Gamma_h}^k - \Delta\Gamma(\mathbf{x}^k)\right]\\ &= \nu\sum_k h^2 e_k\left[(Q^h{\Gamma_h}^k - Q^h\Gamma^k) + (Q^h\Gamma^k - \Delta\Gamma^k)\right]\\ &= \nu(T_1 + T_2)\,,\end{aligned}\tag{4.19}$$

where Q^h is defined in equation (2.7). Write T_1 as

$$\begin{aligned}T_1 &= \sum_k h^2 e_k Q^h e_k\\ &= \frac{1}{\sigma^2}\sum_k h^2 e_k\sum_j h^2 e_j[\Lambda_\sigma(\mathbf{x}^k - \mathbf{x}^j) - \lambda f_\delta(\mathbf{x}^k - \mathbf{x}^j)]\,.\end{aligned}\tag{4.20}$$

From Fourier theory we have that $2\pi\Lambda_\sigma(\mathbf{x}) = \int\hat{\Lambda}_\sigma(\mathbf{s})e^{i\mathbf{s}\cdot\mathbf{x}}d\mathbf{s}$. Therefore, equation (4.20) becomes

$$\begin{aligned}T_1 &= \frac{1}{2\pi\sigma^2}\int\left[\hat{\Lambda}_\sigma(\mathbf{s}) - \lambda\hat{f}_\delta(\mathbf{s})\right]\sum_k h^2 e_k e^{i\mathbf{s}\cdot\mathbf{x}^k}\sum_j h^2 e_j e^{-i\mathbf{s}\cdot\mathbf{x}^j}d\mathbf{s}\\ &= \frac{1}{2\pi\sigma^2}\int\left[\hat{\Lambda}_\sigma(\mathbf{s}) - \lambda\hat{f}_\delta(\mathbf{s})\right]\left|\sum_k h^2 e_k\ e^{i\mathbf{s}\cdot\mathbf{x}(\alpha^k,t)}\right|^2 d\mathbf{s}\,.\end{aligned}$$

Since $\hat{\Lambda}_\sigma(\mathbf{s}) - \lambda\hat{f}_\delta(\mathbf{s}) = \hat{\Lambda}(\sigma\mathbf{s}) - \lambda\hat{f}(\delta\mathbf{s}) = \hat{\Lambda}(c\delta\mathbf{s}) - \lambda\hat{f}(\delta\mathbf{s}) \le 0$ by inequality (4.17), we conclude that

$$T_1 \le 0\,. \tag{4.21}$$

The second term in equation (4.19) is bounded as before, and the remainder of the proof is as in Theorem 4.3. ∎

4.4 Method C and Fishelov's Method

Fishelov [8, 9] has proposed the use of a method that has been generally characterized as related to the PSE method. It is based on discretizations of the equation

$$\frac{\partial \Gamma}{\partial t} + (\mathbf{u} \cdot \nabla)\Gamma = \nu(\Delta g_\sigma * \Gamma)\,, \tag{4.22}$$

where $\Delta\Gamma$ has been approximated by $(\Delta g_\sigma * \Gamma)$ on the right-hand side of equation (1.1), and g_σ is a cutoff function that satisfies $\hat{g}(s) \geq 0$. Fishelov's method is equivalent to method C in the sense that given a cutoff function g_σ one can define functions Λ_σ and f_σ such that $\Delta g_\sigma = \Lambda_\sigma - \lambda f_\sigma$. The reverse is also possible. A natural discretization of the right-hand side of equation (4.22) leads to equation (2.7). As an example consider $g(r)$ of order d (which decays sufficiently fast) and with positive Fourier transform, and define the kernel Λ and new cutoff function f by

$$\Lambda(r) = -\frac{2g'(r)}{r} \quad \text{and} \quad f(r) = -\frac{1}{\lambda}\left[g''(r) + \frac{3g'(r)}{r}\right],$$

respectively, where $\lambda = \int \Lambda(\mathbf{x})d\mathbf{x} = 4\pi g(0)$. One can easily check that Λ is a kernel of order d and f is a cutoff of order $d+2$. The transforms $\hat{\Lambda}(s)$ and $\hat{g}(s)$ are related by the equation $\hat{\Lambda}'(s) = -2s\hat{g}(s)$. Thus we can write

$$\hat{\Lambda}(s) = \hat{\Lambda}(0) - 2\int_0^s \xi \hat{g}(\xi)d\xi\,,$$

which implies that $\hat{\Lambda}(s) \leq \hat{\Lambda}(0)$ whenever $\hat{g}(s) \geq 0$. Moreover, $\hat{\Lambda}(\sigma s) - \lambda\hat{f}(\sigma s) = -\sigma^2 s^2 \hat{g}(s) \leq 0$ so that condition (4.17) is also satisfied.

Cutoff functions with $\hat{f} \geq 0$ are common. For instance, the functions

$$f_1(r) = \frac{1}{\pi}e^{-r^2} \qquad \text{2nd order}$$

$$f_1(r) = \frac{1}{\pi p^2(p^2-1)}\left[p^4 e^{-r^2} - e^{-r^2/p^2}\right] \qquad \text{4th order}$$

have positive Fourier transforms for any $p^2 > 1$. Arbitrarily high-order cutoffs can be derived recursively from the formula

$$f_{n+1}(r) = -\frac{f_n''(r) + 3f_n'(r)/r}{4\pi f_n(0)} \quad \text{for } 1 \leq n\,. \tag{4.23}$$

Their Fourier transforms satisfy

$$\hat{f}_{n+1}(s) = \frac{s^2 \hat{f}_n(s) + 2\int_s^\infty t\hat{f}_n(t)dt}{4\pi \int_0^\infty t\hat{f}_n(t)dt},$$

which are positive as long as the initial one is positive. Infinite-order cutoff functions with positive Fourier transform have also been devised [10].

In Fishelov's method, one starts with a cutoff function g and finds its Laplacian. In method C, one chooses the kernel Λ and the cutoff f and constructs the function $\Lambda - \lambda f$ without knowing which cutoff has a Laplacian equal to this function. A slight advantage of this point of view is that one can construct Laplacians of previously unknown cutoffs. As an example, let

$$\begin{aligned} \Lambda(r) &= \frac{4}{\pi}(3-r^2)e^{-r^2} \\ f(r) &= \frac{1}{\pi p^4(p^4-1)}\left[p^8(2-r^2)e^{-r^2} + (r^2-2p^2)e^{-r^2/p^2}\right]. \end{aligned}$$

The function $\Lambda - \lambda f$ is the Laplacian of the fourth-order cutoff (for $p^2 = 2$)

$$g(r) = \frac{1}{3\pi}\left[5e^{-r^2} - 2e^{-r^2/2} - 2\left(E(1,r^2) - E(1,r^2/2)\right)\right],$$

where $E(x) = \int_1^\infty e^{-xt}t^{-1}\,dt$. Clearly $g(r)$ is not a typical cutoff. Other examples of functions that satisfy the condition in (4.17) for some scaling c are:

- Second order with $c = p > 1$:

$$\begin{aligned} \Lambda(r) &= \frac{4}{\pi}e^{-r^2} \\ f(r) &= \frac{1}{\pi p^2(p^2-1)}\left[p^4 e^{-r^2} - e^{-r^2/p^2}\right] \end{aligned}$$

- Fourth order with $c = 1$ and $p > 1$:

$$\begin{aligned} \Lambda(r) &= \frac{4}{\pi p^4(p^2-1)}\left[p^6 e^{-r^2} - e^{-r^2/p^2}\right] \\ f(r) &= \frac{1}{2\pi}(6 - 6r^2 + r^4)e^{-r^2} \end{aligned}$$

- Sixth order with $c = 1$ and $p > 1$:

$$\begin{aligned} \Lambda(r) &= \frac{4}{\pi p^6(p^4-1)}\left[p^{10}(3-r^2)e^{-r^2} + (r^2-3p^2)e^{-r^2/p^2}\right] \\ f(r) &= \frac{1}{6\pi}(24 - 36r^2 + 12r^4 - r^6)e^{-r^2}. \end{aligned}$$

5 Examples of Kernels Λ

Diffusion kernels Λ for use in the PSE method can be derived from cutoff functions by letting $\Lambda(r) = -2f'(r)/r$, as suggested in [7]. Conditions (C1) through (C3) on f translate into the conditions (K1) through (K3) on Λ, and $\hat{f} \geq 0$ implies (K4).

Fourth-order cutoffs of the form $\Lambda(r) = Ae^{-r^2} + Be^{-r^2/p^2}$ can be constructed with the appropriate choice of constants. For $p^2 > 1$, the function

$$\Lambda(r) = \frac{4}{\pi p^4(p^2-1)}\left[p^6 e^{-r^2} - e^{-r^2/p^2}\right]$$

is an acceptable fourth-order kernel.

We can also find functions of the form $f_{n+1}(r) = P_n(r^2)e^{-r^2}$, where P_n is a polynomial of degree n (see [1]). These cutoffs satisfy the recurrence relation (4.23) with $f_1(r) = e^{-r^2}/\pi$ and thus have positive transform. The closed form of $\Lambda_{n+1}(r)$ derived from these cutoffs is

$$\Lambda_{n+1}(r) = \frac{4}{\pi}e^{-r^2}\sum_{k=0}^{n}(n+1-k)L_k(r^2)\,,$$

where $L_k(x)$ is the Laguerre polynomial of order k. This process leads to kernels of arbitrary order of accuracy. Some examples are given in Table 5.1 and shown in Figure 5.1.

Table 5.1. Examples of high-order diffusion kernels

$\Lambda(r) = \frac{4}{\pi}e^{-r^2}$	2nd order
$\Lambda(r) = \frac{4}{\pi}(3-r^2)e^{-r^2}$	4th order
$\Lambda(r) = \frac{2}{\pi}(12-8r^2+r^4)e^{-r^2}$	6th order
$\Lambda(r) = \frac{2}{3\pi}(60-60r^2+15r^4-r^6)e^{-r^2}$	8th order
$\Lambda(r) = \frac{1}{6\pi}(360-480r^2+180r^4-24r^6+r^8)e^{-r^2}$	10th order

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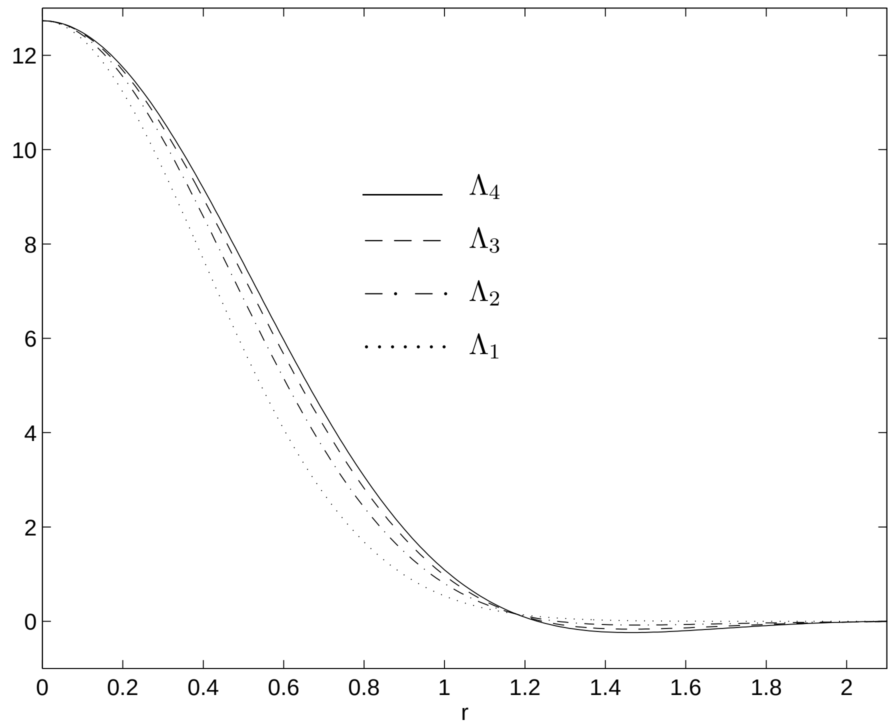

$$\Lambda_1(r) = \frac{4}{\pi\sigma_1^4} e^{-q_1^2}, \quad q_1 = r/\sigma_1$$

$$\Lambda_2(r) = \frac{4}{\pi\sigma_2^4}\left[3 - q_2^2\right] e^{-q_2^2}, \quad q_2 = r/\sigma_2$$

$$\Lambda_3(r) = \frac{2}{\pi\sigma_3^4}\left[12 - 8q_3^2 + q_3^4\right] e^{-q_3^2}, \quad q_3 = r/\sigma_3$$

$$\Lambda_4(r) = \frac{2}{3\pi\sigma_4^4}\left[60 - 60q_4^2 + 15q_4^4 - q_4^6\right] e^{-q_4^2}, \quad q_4 = r/\sigma_4$$

Figure 5.1. Comparison of diffusion kernels Λ of increasing order. Here Λ_k is of order $2k$. The values $\sigma_1^4 = \frac{1}{10}$, $\sigma_2^4 = \frac{3}{10}$, $\sigma_3^4 = \frac{3}{5}$, and $\sigma_4^4 = 1$ were used for the comparisons so that $\Lambda_k(0)$ are all equal.

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Ricardo Cortez
Courant Institute
New York University
251 Mercer Street
New York, NY 10012
E-mail: cortezr@cims.nyu.edu

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