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CONVERGENCE CHARACTERISTICS AND COMPUTATIONAL COST OF TWO ALGEBRAIC KERNELS IN VORTEX METHODS WITH A TREE-CODE ALGORITHM*

D. WEE†, Y. M. MARZOUK‡, F. SCHLEGEL§, AND A. F. GHONIEM§

Abstract. We study the convergence characteristics of two algebraic kernels used in vortex calculations: the Rosenhead–Moore kernel, which is a low-order kernel, and the Winckelmans–Leonard kernel, which is a high-order kernel. To facilitate the study, a method of evaluating particle-cluster interactions is introduced for the Winckelmans–Leonard kernel. The method is based on Taylor series expansion in Cartesian coordinates, as initially proposed by Lindsay and Krasny [J. Comput. Phys., 172 (2001), pp. 879–907] for the Rosenhead–Moore kernel. A recurrence relation for the Taylor coefficients of the Winckelmans–Leonard kernel is derived by separating the kernel into two parts, and an error estimate is obtained to ensure adaptive error control. The recurrence relation is incorporated into a tree-code to evaluate vorticity-induced velocity. Next, comparison of convergence is made while utilizing the tree-code. Both algebraic kernels lead to convergence, but the Winckelmans–Leonard kernel exhibits a superior convergence rate. The combined desingularization and discretization error from the Winckelmans–Leonard kernel is an order of magnitude smaller than that from the Rosenhead–Moore kernel at a typical resolution. Simulations of vortex rings are performed using the two algebraic kernels in order to compare their performance in a practical setting. In particular, numerical simulations of the side-by-side collision of two identical vortex rings suggest that the three-dimensional evolution of vorticity at finite resolution can be greatly affected by the choice of the kernel. We find that the Winckelmans–Leonard kernel is able to perform the same task with a much smaller number of vortex elements than the Rosenhead–Moore kernel, greatly reducing the overall computational cost.

Key words. numerical simulation, convergence, computational particle methods, vortex methods, tree-code, N-body problems, hierarchical methods

AMS subject classifications. 65M12, 65N12, 76M23

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1. Introduction. The evaluation of interparticle interactions in Lagrangian vortex methods forms a classical N-body problem, whose computational cost scales as $O(N^2)$. This cost is prohibitive for large-scale, three-dimensional computations. To alleviate this difficulty, fast summation algorithms have been proposed [2, 3, 8, 19].

In many of these approaches, particles are divided into a nested set of clusters, and particle-particle interactions are replaced by particle-cluster interactions, which can be efficiently evaluated by using an expansion. Such tree-code algorithms reduce the operation count to $O(N \log N)$ or even to $O(N)$.

Among various fast summation algorithms, the tree-code algorithm developed by Lindsay and Krasny [11] was utilized to perform some of our previous simulations [12, 13, 20]. In this method, particle-cluster interactions are evaluated by using Taylor

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series expansion of the Rosenhead–Moore kernel [14, 15], i.e., the low-order algebraic
kernel [21]. The expansion is carried up to the 8th order, and the Taylor coefficients
are computed using a recurrence relation. The use of a recurrence relation reduces the
computational cost of performing high-order expansions, enabling the use of coarse
clusters. A parallel version of the code was also developed and successfully used for
large-scale calculations [12, 13]. The algorithm has been extended to evaluate not only
the velocity induced by vorticity, but also the velocity induced by volume sources and
the gradients of these velocity fields to simulate buoyant flows [16].

The status of the Rosenhead–Moore kernel, however, is somewhat controversial.
While, from many previous applications, it is generally believed that the kernel pro-
vides convergence in all cases of practical interest, it has been warned that the kernel
does not satisfy an inequality required in the classical proof of convergence of vortex
methods [21]. Additionally, even if it does lead to convergence, the convergence rate
is expected to be lower than that of the transcendental kernel based on the Gaussian
core function, since the kernel is constructed from a low-order core function. To ad-
dress these issues, Winckelmans and Leonard [21] introduced a higher-order algebraic
kernel, which we shall call the Winckelmans–Leonard kernel in this article. The kernel
satisfies all the requirements in the classical convergence analysis of vortex methods,
and is expected to be more numerically convenient than those kernels involving tran-
scendental functions. However, actual evaluation of the benefit of this new kernel over
the low-order one has never been explicitly performed.

In this context, this article presents two interrelated results. First, we present a
tree-code to evaluate the velocity field for the Winckelmans–Leonard kernel. The tree-
code algorithm itself bears similarity to the one previously introduced by Lindsay and
Krasny [11], but utilizes a different recurrence relation suitable for the Winckelmans–
Leonard kernel. Next, we compare the two algebraic kernels, utilizing the tree-code.
Evaluation of the velocity field from a Gaussian vorticity distribution and calculations
of vortex rings at intermediate Reynolds numbers are presented. The former exam-
ple yields numerical estimates of convergence rates, and the latter example provides
insights into the effect of different kernels in practical applications.

The article is organized as follows. In section 2, we start by briefly describing the
exposition more self-contained. Next, a new recursive method to evaluate the Taylor
coefficients of the Winckelmans–Leonard kernel is presented. Finally, in section 3,
the tree-code is utilized to investigate the convergence properties of the Rosenhead–
Moore kernel and the Winckelmans–Leonard kernel. Both theoretical and numerical
discussion is provided. We show that both algebraic kernels lead to convergence, with
the Winckelmans–Leonard kernel exhibiting the superior convergence rate. A brief
summary follows at the end.

2. Description of the adaptive tree-code. In this section, our tree-code al-
gorithm is described. The tree-code algorithm for the Rosenhead–Moore kernel, which
was developed by Lindsay and Krasny [11], is first summarized. The exposition of
the previous development is made only for ease of reference. Then, the new recur-
sive method of evaluating the Taylor coefficients of the Winckelmans–Leonard kernel is
presented. A numerical example is provided to show the performance of the tree-code.

of our interest is stated as follows. For each time step during vortex simulations, it is
necessary to invert the following equation:

\[ \omega = \nabla \times u. \]  

That is, knowing the vorticity field \( \omega \), we need to calculate the velocity field \( u \). \( \omega \) is discretized into Lagrangian computational elements or particles:

\[ \omega(x) \approx \sum_{j=1}^{N} W_j f_{\sigma}(x - y_j). \]  

\( f_{\sigma} \) is a radially symmetric core function of radius \( \sigma \), given by \( f_{\sigma}(x) \equiv \sigma^{-3} f(|x|/\sigma) \). In \( \mathbb{R}^3 \), the solution of (2.1) is given by the Biot–Savart law:

\[ u(x) = -\frac{1}{4\pi} \int \frac{x - y}{|x - y|^3} \times \omega(y) dy \approx \sum_{j=1}^{N} K_{\sigma}(x, y_j) \times W_j, \]  

where \( K_{\sigma} \) is given by

\[ K_{\sigma}(x, y) = -\frac{1}{4\pi} \int \frac{x - z}{|x - z|^3} f_{\sigma}(z - y) dz. \]  

To evaluate (2.3), a tree is constructed. Computational particles are divided into a nested set of clusters, and particle-particle interactions are replaced by a smaller number of particle-cluster interactions. The tree construction starts with the root cell containing all the particles. The cell on the next level is obtained by bisecting one of the cells at the current level in one of three coordinate directions. When every terminal cell in the tree contains a number of particles smaller than the predefined leaf size, \( N_0 \), which is predefined by the user, the process terminates and returns the tree structure. Once the tree is constructed, (2.3) is rewritten in the following form:

\[ u(x) = \sum_{c} \sum_{j=1}^{N_c} K_{\sigma}(x, y_j) \times W_j, \]  

where \( c \) denotes a cluster containing \( N_c \) particles. Each particle-cluster interaction is evaluated using either a Taylor approximation or a direct summation. The procedure uses a complex combination of theoretical error estimates and empirical computational time estimates to determine the best order of the approximation and the best size of the cluster.

To derive the Taylor approximation for a particle-cluster interaction, \( K_{\sigma}(x, y) \) in (2.5) is expanded in the Taylor series with respect to \( y \), around the cluster center \( y_c \), such that

\[ \sum_{j=1}^{N_c} K_{\sigma}(x, y_j) \times W_j = \sum_{k} a_k(x, y_c) \times m_k(c). \]  

Here, \( a_k(x, y_c) \) is the \( k \)th Taylor coefficient of \( K_{\sigma}(x, y) \) at \( y_c \):

\[ a_k(x, y_c) = \frac{1}{k!} \partial_y^k K_{\sigma}(x, y_c), \]
and \( m_k(c) \) is the \( k \)th moment of the vortex elements in cluster \( c \) about its center \( \mathbf{y}_c \):

\[
(2.8) \quad m_k(c) = \sum_{j=1}^{N_c} W_j(y_j - y_c)^k.
\]

\( k = (k_1, k_2, k_3) \) is an integer multi-index with \( k_i \geq 0 \), and \( k! = k_1! k_2! k_3! \). For \( x \in \mathbb{R}^3 \), \( x^k \) and \( D^m_y \) are interpreted in the standard way; i.e., \( x^k = x_1^{k_1} x_2^{k_2} x_3^{k_3} \) and \( D^m_y = D^{n_1}_y D^{n_2}_y D^{n_3}_y \), where \( D_{yi} = \frac{\partial}{\partial y_i} \). The infinite series in (2.6) is approximated by a finite sum,

\[
(2.9) \quad \sum_{j=1}^{N_c} K_\sigma(x, y_j) \times W_j \approx \sum_{|k|<p} a_k(x, y_c) \times m_k(c),
\]

where \( |k| = k_1 + k_2 + k_3 \). The order of the approximation, \( p \), must be chosen so that the error due to truncation remains small. To evaluate (2.9), we need the Taylor coefficients, i.e., \( a_k \). We define a scalar potential, \( \phi_\sigma \), which yields the kernel, \( K_\sigma \), as its gradient:

\[
(2.10) \quad K_\sigma(x, y) = -\nabla_y \phi_\sigma(x, y).
\]

We set the \( k \)th Taylor coefficient of \( \phi_\sigma(x, y) \) at \( y = y_c \) as follows:

\[
(2.11) \quad T_k(x, y_c) = \frac{1}{k!} D^k_y \phi_\sigma(x, y_c).
\]

Then, \( a_k \) is related to \( T_k \) as follows:

\[
(2.12) \quad a_k(x, y_c) = -\sum_{i=1}^{3} \hat{e}_i (k_i + 1) T_{k+i}(x, y_c),
\]

where \( \hat{e}_i \) is the \( i \)th Cartesian-basis vector. Therefore, to compute \( a_k \), it is sufficient to obtain \( T_k \). For the Rosenhead–Moore kernel:

\[
(2.13) \quad K^{RM}_\sigma(x, y) = -\frac{1}{4\pi} \frac{x - y}{(|x - y|^2 + \sigma^2)^{3/2}},
\]

the potential is the Plummer potential:

\[
(2.14) \quad \phi^{RM}_\sigma(x, y) = \frac{1}{4\pi} \frac{1}{(|x - y|^2 + \sigma^2)^{1/2}}.
\]

The calculation of the corresponding \( T_k \) is performed recursively, using the following formula [11]:

\[
(2.15) \quad |k| R^2 T_k - (2|k| - 1) \sum_{i=1}^{3} (x - y) \cdot \hat{e}_i T_{k-\hat{e}_i} + (|k| - 1) \sum_{i=1}^{3} T_{k-2\hat{e}_i} = 0,
\]

for \( |k| \geq 1 \), where \( T_0(x, y_c) = \phi_\sigma(x, y_c) \), \( T_k(x, y_c) = 0 \) if any \( k_i < 0 \), and \( R = \sqrt{|x - y_c|^2 + \sigma^2} \).

Further details of the tree-code can be found in the work by Lindsay and Krasny [11].
2.2. Extension to the Winckelmans–Leonard kernel. The high-order algebraic kernel, or equivalently the Winckelmans–Leonard kernel, is given as follows [21]:

\[
K^W_L(x, y) = -\frac{1}{4\pi} \frac{|x - y|^2 + \frac{3}{2} \sigma^2}{(|x - y|^2 + \sigma^2)^{3/2}} (x - y).
\]

The corresponding potential is given by

\[
\phi^W_L(x, y) = \frac{1}{4\pi} \frac{|x - y|^2 + \frac{3}{2} \sigma^2}{(|x - y|^2 + \sigma^2)^{3/2}}.
\]

One way to compute the Taylor coefficients of the Winckelmans–Leonard kernel is to split \(\phi^W_L(x, y)\) into two parts and to develop a recurrence relation for each part separately; i.e.,

\[
\phi^W_L(x, y) = \frac{\phi^1_0(x, y)}{4\pi} + \frac{\sigma^2 \phi^3_0(x, y)}{8\pi},
\]

where \(\phi^1_0(x, y) = (|x - y|^2 + \sigma^2)^{-\nu/2}\). Note that \(\phi^R_M = \phi^1_0/4\pi\). That is, the potential for the Winckelmans–Leonard kernel can be obtained by adding a correction term to the Plummer potential. The recurrence relation for the Taylor coefficients of \(\phi^\nu_\sigma\) for each \(\nu\) is already available [6]. Setting

\[
T^\nu_n = T^\nu_n(x, y) = \frac{1}{n!} D^\nu_n \phi^\nu_\sigma(x, y),
\]

it has been shown that

\[
|n|(|x - y|^2 + \sigma^2)T^\nu_n - (2|n| + \nu - 2) \sum_{i=1}^{3} (x_i - y_i)T^\nu_n = 0.
\]

Once knowing \(T^1_n\) and \(T^3_n\), the Taylor coefficients of \(\phi^W_L(x, y)\) can be obtained by taking the sum

\[
T_n = \frac{T^1_n}{4\pi} + \frac{\sigma^2 T^3_n}{8\pi}.
\]

Using (2.21), we write

\[
\sum_{j=1}^{N_c} \phi^W_L(x, y_c)W_j \approx \frac{1}{4\pi} \sum_{|n| < p} T^1_n(x, y_c)m_n(c)
\]

\[
+ \frac{\sigma^2}{8\pi} \sum_{|n| < p} T^3_n(x, y_c)m_n(c).
\]

To estimate the error in (2.22), we write the sum of the neglected terms as follows:

\[
\frac{1}{4\pi} \sum_{|n| \geq p} T^1_n(x, y_c)m_n(c) + \frac{\sigma^2}{8\pi} \sum_{|n| \geq p} T^3_n(x, y_c)m_n(c)
\]

\[
= \frac{1}{4\pi} \sum_{n \geq p} \sum_{j=1}^{N_c} B^1_n(x, y_c, y_j)W_j + \frac{\sigma^2}{8\pi} \sum_{n \geq p} \sum_{j=1}^{N_c} B^3_n(x, y_c, y_j)W_j,
\]
where

\[ B^\nu_n(x, y_c, y_j) = \sum_{|k|=n} T^\nu_k(x, y_c)(y_j - y_c)^k. \]

Multiplying (2.20) by \((y_j - y_c)^n\) and summing over all indices \(n\) with \(|n| = n\), we obtain

\[ nR^2B^\nu_n - (2n + \nu - 2)\alpha B^\nu_{n-1} + (n + \nu - 2)\beta^2 B^\nu_{n-2} = 0, \]

where \(\alpha = (x - y_c)(y_j - y_c)\), and \(\beta = |y_j - y_c|\). As discussed in [6], (2.25) is similar to the recurrence relation of the Gegenbauer polynomials [1]:

\[ nC^{(\nu/2)}_n(x) - (2n + \nu - 2)xC^{(\nu/2)}_{n-1}(x) + (n + \nu - 2)C^{(\nu/2)}_{n-2}(x) = 0. \]

Comparing (2.25) and (2.26), we conclude that

\[ B^\nu_n(x, y_c, y_j) = \frac{1}{R^\nu} \left( \frac{\beta}{R} \right)^n C^{(\nu/2)}_n(\alpha/\beta R). \]

Note that \(|\alpha/\beta R| \leq 1\), and that

\[ \forall |x| \leq 1, \quad |C^{(\nu/2)}_n(x)| \leq \frac{(n + \nu - 1)!}{n!(\nu - 1)!}. \]

Hence,

\[ |B^1_n(x, y_c, y_j)| \leq \frac{1}{R} \left( \frac{|y_j - y_c|}{R} \right)^n, \]

and

\[ |B^3_n(x, y_c, y_j)| \leq \frac{n + 2)(n + 1)}{2R^3} \left( \frac{|y_j - y_c|}{R} \right)^n. \]

We take the first term of the series in (2.23) as a heuristic estimate of the error. With (2.29) and (2.30), the estimated error, \(E_p\), becomes

\[ E_p = \frac{M_p(c)}{4\pi R^{p+1}} \left( 1 + \frac{(p + 2)(p + 1)}{2} \frac{\sigma^2}{R^2} \right), \]

where

\[ M_p(c) = \sum_{j=1}^{N_c} |y_j - y_c| |W_j|. \]

Since \(M_p(c) \leq M_0(c)r^p\), where \(r\) represents the radius of the cluster \(c\), the asymptotic behavior of the error is given by

\[ E_p = O(h^p) + O(p^2h^p\eta^2), \]

where \(h = r/R\), and \(\eta = \sigma/R\), as \(h \to 0\), \(\eta \to 0\), and \(p \to \infty\).
2.3. Numerical results. The method described in the previous section has been incorporated into the tree-code originally developed by Lindsay and Krasny [11]. We now compute the velocity field induced by two colliding vortex rings, whose particle distribution is shown in Figure 1, to test the new tree-code with the higher-order kernel. The rings consist of 163,251 particles, and the velocity field is evaluated on a uniform rectangular grid encompassing the particles. The number of grid points is 96,000. The total number of particle-grid point interactions is roughly $1.57 \times 10^{10}$.

The expansion, expressed by (2.9), (2.12), and (2.21) with (2.20) and its variants, is used to compute the velocity field when the following criterion is met:

$$4\pi E_p = \frac{M_p(c)}{R^{n+1}} \left( 1 + \frac{(p+2)(p+1)}{2} \frac{\sigma^2}{R^2} \right) \leq \epsilon,$$

where $\epsilon$ is a user-defined parameter. This criterion is derived from (2.31). We set $N_0 = 64$ and $\sigma = 0.1$. The maximum order of the expansion is limited to 8. The calculation is performed with double precision on a Pentium 4 workstation. Figure 2 shows the error in the velocity field versus $\epsilon$. The absolute error is defined as follows:

$$E_{\text{abs}} = \max |u_{\text{sum}}(x) - u_{\text{app}}(x)|.$$

The subscript “sum” denotes direct summation, while the subscript “app” denotes tree-code approximation. It is important to distinguish $E_{\text{abs}}$ from the error discussed in section 3. $E_{\text{abs}}$ is just the error induced by the tree-code approximation, which does not include the other sources of error, that is, desingularization and discretization. We also plot the relative error, which is given by

$$E_{\text{rel}} = \max \frac{|u_{\text{sum}}(x) - u_{\text{app}}(x)|}{|u_{\text{sum}}(x)|}.$$

The term “interaction” may be misleading, because there exist only unilateral contributions from vortex elements to grid points. We clarify that one interaction is just the contribution of a vortex element to the velocity at a grid point.
The error varies linearly with $\epsilon$, implying that (2.34) provides reasonable error control. The computational time is also shown in Figure 2. $t_{\text{sum}}$ represents the computational time for direct summation, which is 1,800 seconds in this case. $t_{\text{app}}$ is the computational time for the same job with the tree-code approximation. We plot $t_{\text{app}}/t_{\text{sum}}$, since $t_{\text{app}}$ and $t_{\text{sum}}$ by themselves may vary significantly from one machine to another. The result shows that we achieve $E_{\text{abs}} \approx 10^{-6}$ with slightly more than 10% of the computational time required for direct summation. We note that, for the same example, the Rosenhead–Moore kernel shows behavior very similar to that shown here for the Winckelmans–Leonard kernel. In summary, the overall computational performance of the new tree-code is comparable to that of the original tree-code for the Rosenhead–Moore kernel [11].

Before closing section 2, we note that kernel-independent fast multipole algorithms have recently been introduced [7, 22]. These algorithms may well replace the tree-code described here. However, the result presented in this article is the first reported application of a fast summation routine to the Winckelmans–Leonard kernel, to the authors’ knowledge.

3. Convergence characteristics of the two algebraic kernels. In this section, the convergence characteristics of the two algebraic kernels, that is, Rosenhead–Moore kernel and the Winckelmans–Leonard kernel, are compared. While both kernels lead to convergence, a higher rate of convergence is achieved with the Winckelmans–Leonard kernel.

3.1. On the convergence of the Rosenhead–Moore kernel. Each of the kernels we have investigated so far can be generated from a radially symmetric core function, as shown in (2.4). For the Rosenhead–Moore kernel, the corresponding core function is given by

\[ f^{\text{RM}}(\rho) = \frac{3}{4\pi} \frac{1}{(\rho^2 + 1)^{5/2}}. \]
On the other hand, the core function for the Winckelmans–Leonard kernel is given by

\[ f^{WL}(\rho) = \frac{15}{8\pi} \frac{1}{(\rho^2 + 1)^{7/2}}. \]

Since the core function for the Rosenhead–Moore kernel has relatively slow decay at infinity, the following inequality is not satisfied by the Rosenhead–Moore kernel:

\[ \exists d \geq 2, \text{ such that (s.t.) } \int_0^\infty |f(\rho)|\rho^{2+d}d\rho < \infty. \]

Citing the study by Cottet [4], Winckelmans and Leonard [21] have warned that the Rosenhead–Moore kernel may not lead to convergence due to the lack of this inequality. Since numerical experiments with the kernel show quantitatively accurate results [20], it is of importance to check whether such a danger of nonconvergence truly exists.

Tracing the proof in [4], it is found that the only major place where the inequality (3.3) appears is Item (iv) in Lemma 5.4 of [4], which is restated here as follows.

Assuming that

\[ \int f(|x|)dx = 1, \]
\[ \int x^k f(|x|)dx = 0, \quad 1 \leq |k| < d - 1, \quad \text{and} \]
\[ \int |x|^d |f(|x|)|dx < \infty, \]

we get

\[ ||(K - K_\sigma) \ast T||_{0,p} \leq C \sigma^d (||T||_{d,1} + ||T||_{d,\infty}), \]

if \( T \in W^{d,\infty}(\mathbb{R}^3) \cap W^{d,1}(\mathbb{R}^3) \), and

\[ ||(K - K_\sigma) \ast T||_{0,p} \leq C \sigma^d ||T||_{d-1,p}, \]

if \( T \in W^{d-1,p}(\mathbb{R}^3) \), \( 1 < p < \infty \).

Here, the following notation is used:

\[ (F \ast G)(x) \equiv \int_{\mathbb{R}^3} F(x, y) \times G(y)dy, \quad \text{and} \]
\[ K(x, y) = \frac{1}{4\pi} \frac{x - y}{|x - y|^3}. \]

In particular, (3.6) corresponds to (3.3). The inequality is used to show that the error of desingularization behaves in a consistent way. The other part of the error, i.e., the error of discretization, behaves independently from the inequality. It has not been explicitly stated in [4] that \( d \geq 2 \). The condition of \( d \geq 2 \) turns out to be necessary, however, for developing (3.8). Here we suggest that the statement can be modified to include the case of \( d = 1 \). This is of particular importance, since, if \( d \) is taken to be 1,
the Rosenhead–Moore kernel does satisfy all the requirements. Given a test function \( \phi \), we use integration by parts to get

\[
\left| \int (T - f_\sigma \ast T)(x) \, \phi(x) dx \right| \\
= \left| \int \left( \int_{t=0}^{1} \int z \cdot \nabla T(x + tz) f_\sigma(z) dz \, dt \right) \phi(x) dx \right| \\
\leq C \|T\|_{1,p} \|\phi\|_{1,p'} \int |z| f_\sigma(z) dz \\
\leq C \sigma \|T\|_{1,p} \|\phi\|_{1,p'},
\]

where \( 1/p + 1/p' = 1 \). Thus, \( \|T - f_\sigma \ast T\|_{-1,p} \leq C \sigma \|T\|_{1,p} \). After this distribution estimate is established, (3.8) simply follows from the Calderon’s theorem [5]:

\[
\|K \ast (T - f_\sigma \ast T)\|_{0,p} \leq C \|T - f_\sigma \ast T\|_{-1,p} \leq C \sigma \|T\|_{1,p}.
\]

With this last inequality, we modify (3.8) as follows:

\[
\| (K - K_\sigma) \ast T \|_{0,p} \leq C \sigma^{d} \|T\|_{d-1,p},
\]

if \( T \in W^{d-1,p}(\mathbb{R}^3), 1 < p < \infty, d' = \max(d, 2) \). Equation (3.13) is valid for \( d \geq 1 \), and this should be sufficient for the further development of the convergence analysis given in [4]. For instance, Lemma 5.5 in [4] can be proven for the Rosenhead–Moore kernel, if enough regularity is guaranteed for the initial vorticity field \( \omega \) to ensure that \( \omega \) behaves as \( O(\sigma) \) for the Rosenhead–Moore kernel. On the other hand, the Winckelmans–Leonard kernel satisfies (3.8) with \( d = 2 \), and hence its desingularization error should behave as \( O(\sigma^2) \).

3.2. Numerical comparison between the two algebraic kernels. The error discussed in the previous subsection includes the error due to desingularization only. However, the error due to desingularization becomes a meaningful estimate of the overall error only for the case where the error due to discretization is small. In practice, one performs simulations, while keeping the overlap ratio, i.e., \( \sigma / \Delta x \), approximately constant. In such a case, the apparent convergence rate may be different from that predicted by analysis. As a practical guide, three numerical examples are provided in this section. In the first example, we compute a velocity field induced by a Gaussian vorticity distribution, whose exact solution is known, to perform a convergence study. The second example deals with the temporal evolution of a vortex ring, which includes many of the additional complications—a time-evolving particle distribution, diffusion, remeshing—that arise in practical vortex calculations. The last example is the side-by-side collision of two identical vortex rings, which concerns three-dimensional distortion of vorticity. It turns out that the three-dimensional evolution at finite resolution is pretty sensitive to the choice of the kernel, while the subtle difference can be obscured in more symmetric cases.
3.2.1. Gaussian vorticity distribution. Using two algebraic kernels, we compute the velocity field induced by a Gaussian distribution:

\[ T(x) = \frac{\mathbf{e}_2}{(2\pi)^{3/2}} e^{-|x|^2/2}. \]

The velocity field induced by this vorticity distribution is exactly

\[ u(x) = (K \ast T)(x) = -\frac{x \times \mathbf{e}_2}{4\pi|x|^3} \left( \text{erf} \left( \frac{|x|}{2^{1/2}} \right) - \left( \frac{2}{\pi} \right)^{1/2} |x| e^{-|x|^2/2} \right). \]

Due to the azimuthal symmetry of the distribution, one may just compute the velocity on a plane, e.g., \( x_3 = 0 \) in this case, to estimate the error in \( \mathbb{R}^3 \). Since it is apparent that the maximum error should be found along the line of \( x_2 = 0 \) in this plane, where high velocity occurs, we compute only the velocity on that line. Furthermore, with a few calculations at coarse resolution, we have found that the maximum error actually occurs near \( x_1 = 1 \). Thus, we concentrate our velocity computations on the line segment \( x_1 \in [0, 1.5], x_2 = x_3 = 0 \). Among three components of the velocity field, i.e., \( u_1, u_2, \) and \( u_3 \), only \( u_3 \) is nontrivial on this line, and hence only \( u_3 \) is reported. Such a simplification is necessary to realize calculations at a resolution fine enough to obtain converging behaviors.

The distribution in (3.14) is not of compact support. However, it exponentially decays at infinity, and we may specify a reasonable cutoff distance: numerical discretization of the vorticity field is made only for \( -4 \leq x_i \leq 4 \). Within the domain of discretization, we place a uniform grid with resolution discretized distribution as follows:

\[ T(x) = \sum_j T(x_j) \Delta x^3 \delta(x - x_j), \]

where the index \( j \) runs over all the grid points. The discretized velocity field is recovered by taking

\[ u^{RM}(x) = (K^{RM}_\sigma \ast T)(x), \]
\[ u^{WL}(x) = (K^{WL}_\sigma \ast T)(x), \]

where \( K^{RM}_\sigma \) and \( K^{WL}_\sigma \) are defined in section 2. The calculation is performed by the tree-code discussed in the previous section with \( \epsilon = 0.0005 \) and \( N_0 = 64 \). The computation is performed as \( \Delta x \) is refined while \( \sigma/\Delta x \) is kept equal to 2. This is a typical overlap ratio reported previously to be effective [10].

The overall convergence rate is estimated by refining \( \Delta x \). Results are shown in Figure 3, where the error is plotted against \( \Delta x \). The error associated with the Winckelmans–Leonard kernel indeed decays faster than that of the Rosenhead–Moore kernel. The rate of convergence for the Rosenhead–Moore kernel is around \( O(\sigma^{1.75}) \). The rate of convergence for the Winckelmans–Leonard kernel turns out to be \( O(\sigma^2) \), which is higher than that of the Rosenhead–Moore kernel, though not higher by one order as expected from the previous analysis. Nevertheless, the absolute velocity error is much smaller with the Winckelmans–Leonard kernel than with the Rosenhead–Moore kernel; for a typical resolution, switching from the Rosenhead–Moore kernel to the Winckelmans–Leonard kernel provides an order-of-magnitude reduction in the error, and this difference becomes even greater as the resolution increases.
3.2.2. Evolution of a vortex ring. In this second example, we study the evolution of a single vortex ring. A ring of radius $R$ and core radius $a$ is initially placed at the $x_2 = 0$ plane. The core of the ring is represented by its azimuthal vorticity distribution:

\begin{equation}
\omega_\phi = \frac{K \Gamma}{\pi a^2} \exp \left[ -K \left( \frac{R^2}{a^2} + \frac{r^2}{a^2} - \frac{2Rr}{a^2} \sin \theta \right) \right],
\end{equation}

where $r = \sqrt{x_1^2 + x_2^2 + x_3^2}$, $\tan \theta = (\sqrt{x_1^2 + x_3^2})/x_2$, and $K = (2.24182)^2/4$. To make the initial distribution smooth, an image ring was placed across the axis of symmetry so that $\omega_\phi = 0$ at the $x_2$ axis. The ring has unit circulation and unit radius, i.e., $\Gamma = 1$ and $R = 1$. We set $Re_\Gamma = \Gamma/\nu = 500$. The ring’s core radius is chosen to be $a/R = 0.35$. This set of parameters makes the initial condition identical to that of a previous axisymmetric spectral simulation reported in [17, 18] and to that of other vortex calculations reported in [16, 20]. The initial condition is discretized on a relatively fine grid whose mesh size is $\Delta x = 0.025$.

The numerical discretization of the equation of motion closely follows that of [16]. A second-order predictor/corrector scheme is used for evaluating advection. Viscosity is implemented by utilizing the interpolation kernel $\Lambda_3$ [20]. Three distinct cases are reported. Case I uses the Rosenhead–Moore kernel with a time step of $\Delta t = 0.5$, a core size of $\sigma = 0.1$, and a mesh size for interpolation of $\Delta x = 0.05$. Vortex elements with $|W_j| < 10^{-8}$ are eliminated to control the size of the problem at the end of each time step. Case II has discretization parameters identical to those in Case I, but uses the Winckelmans–Leonard kernel instead of the Rosenhead–Moore kernel. Finally, a coarser simulation with the Winckelmans–Leonard kernel is presented as Case III, where $\sigma = 0.2$ and $\Delta x = 0.1$. All the cases share the same value of $\sigma/\Delta x$—the overlap ratio is constant. The number of elements in Case III is expected to be about $1/8$ of that in Case I, since $\Delta x$ is doubled. All the calculations have been performed by using 16 cores in a computing cluster built with quad-core Xeon processors at either 2.33 GHz or 2.66 GHz. Parallelization is done in a similar way to that discussed in [12].
The results are reported in the following dimensionless variables, which were also used in previous related works [16, 17, 18, 20]. The dimensionless speed of the vortex ring centroid is given by

\[ \overline{U} = U_c \left( \frac{I_0}{\rho} \right)^{1/2} \left( \nu \right)^{3/2}, \]  

where \( I_0/\rho \) is the initial linear impulse of the ring and \( U_c \) is the centroid speed measured in the computational units. We also use dimensionless time, which is scaled as

\[ \tau = \frac{t \nu^2}{I_0/\rho}, \]

and shifted to match the initial time reported in [17, 18].

Figure 4 shows the speed of the vortex ring centroid. While all the vortex ring calculations underestimate the speed of the vortex ring compared to the value reported by [17, 18] due to limited resolution, we find a sizable improvement in Case II over Case I, implying that the Winckelmans–Leonard kernel indeed provides a much more accurate description of the evolution and deformation of the vortex ring. Even Case III, whose resolution is much coarser, exhibits a speed comparable to that of Case I. The difference is also detectable in qualitative pictures of vorticity evolution. Figure 5 shows the contour lines of \(|\omega_z|\) on the plane of \( z = 0 \) at \( \tau = 10.03 \times 10^{-5} \). Case I is shown for \( x > 0 \) (top), while Case II is shown for \( x < 0 \) (bottom). Due to the difference in centroid speeds, the vortex ring in Case II is observed at a location slightly ahead of that in Case I. The elongated tail of the vortex ring, captured at much finer resolutions in [16, 17, 18, 20], is also reproduced in Case II, while Case I truncates this subtle feature.

The wall clock time for evaluating advection per time step is given in Figure 6 to provide a sense of the relative computational efforts. From the figure, it is clear that...
Fig. 5. Contour of $|ω_ζ|$ on the plane of $z = 0$ at $t = 10.03 \times 10^{-5}$. Case I is shown in $x > 0$ (top), while Case II is shown in $x < 0$ (bottom). The levels of thin lines vary from $|ω_ζ| = 0.024$ to $|ω_ζ| = 0.24$, incrementally by 0.024. The levels of thick lines start from $|ω_ζ| = 0.24$ at the outermost one, and increase by 0.24 in every interval. The innermost thin line and the outermost thick line collapse onto each other in each case.

Case II is a more demanding simulation than Case I; the accuracy of the Winckelmans–Leonard kernel does not come free. However, by comparing Case III with Case I, we can see that the benefit outweighs this additional cost. Case III reproduces the vortex ring speed at the same level of accuracy as Case I, utilizing only a fraction of the vortex elements (less than 20%). Though the evaluation of each pair-wise interaction with the Winckelmans–Leonard kernel tends to be more expensive than with the Rosenhead–Moore kernel, use of the Winckelmans–Leonard kernel greatly reduces the overall computational cost—in terms of both CPU time and memory—by allowing a much smaller number of elements to perform the same task.

3.2.3. Interaction of two vortex rings: Side-by-side collision. The final numerical example is the interaction of two vortex rings; the case was studied earlier in [9, 20]. Two identical vortex rings are initially placed side-by-side. The centers of the vortex rings lie on the $x$-axis, separated by a distance $s$. The radius of each ring
Parameters used for each case of colliding vortex rings. \( \Delta x_0 = 0.990909 \), \( \sigma_0 = 0.2 \), and \( \Delta t_0 = 0.05 \). Cases whose names start with RM use the Rosenhead–Moore kernel, while those with WL use the Winckelmans–Leonard kernel.

<table>
<thead>
<tr>
<th>Case</th>
<th>( \Delta x_0 / \Delta x = \sigma_0 / \sigma )</th>
<th>( \Delta t_0 / \Delta t )</th>
</tr>
</thead>
<tbody>
<tr>
<td>RM1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>RM2</td>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td>WL1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>WL2</td>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td>WL3</td>
<td>( 2\sqrt{2} )</td>
<td>8</td>
</tr>
<tr>
<td>WL4</td>
<td>4</td>
<td>16</td>
</tr>
</tbody>
</table>

is \( \mathcal{R} \). We use a Gaussian vorticity distribution with the core

\[
\omega_\phi = \omega_0 \exp \left[ -\left( \frac{r}{a} \right)^2 \right],
\]

where \( r \) is the distance from the core centerline, and \( \omega_0 \) is the maximum vorticity at the core center. The expression (3.22) is identical to (3.19) with a proper change of variables. We study the case with \( \mathcal{R} = 0.982 \), \( a = 0.393 \), \( s = 3.65 \), \( \omega_0 = 23.8 \), and \( \nu = 0.01 \). The rings are perfectly aligned on the \( y = 0 \) plane, without any out-of-plane inclination.}

Six cases are investigated, whose numerical parameters are summarized in Table 1. Time advance is performed by the same algorithm utilized in section 3.2.2 with a time interval of \( \Delta t = \Delta t_c = \Delta t_d \), while the mesh size for interpolation is given by \( \Delta x \). The core size \( \sigma \) is kept proportional to \( \Delta x \) to keep the overlap ratio constant. The same computing facility as described in section 3.2.2 is used, with a similar set of task geometries.

The overall motion of the vortex rings can be summarized as follows: both rings travel in the positive \( y \) direction, while their mutual induction introduces significant distortion. The rings approach each other, and collide along the \( x = 0 \) plane. Viscous dissipation is enhanced by the collision, and the two rings eventually merge into a highly distorted single ring. This overall behavior is captured by both kernels at the lowest resolution (RM1 and WL1), as shown by the vorticity magnitude isosurfaces in Figure 7. Two distinct differences are, however, clear. First, the rings of WL1 travel faster than those of RM1. The difference in the speed of motion is quantitatively confirmed by Figure 8, where we plot the centroid speed of the vortex rings in all the cases. The initial speeds of the centroid in WL1 and WL2 are significantly higher than those in RM1 and RM2, resulting in faster evolution. The refined calculation with the Rosenhead–Moore kernel (RM2) closely follows the result of the calculation with the Winckelmans–Leonard kernel at the lowest resolution (WL1). Refinement within the cases where the Winckelmans–Leonard kernel is used, on the other hand, shows only minor improvements, as one can see from the small differences among the curves representing WL2, WL3, and WL4. These observations suggest that the approximate solutions from the Winckelmans–Leonard kernel already exhibit a well-converging solution, and indeed are more accurate than those from the Rosenhead–Moore kernel at the same resolution. Second, three-dimensional distortion at \( t = 5 \) (e.g., in

\[\text{Though the initial condition is similar to that of [9], it is not exactly identical in the sense that our rings are isolated in space while the case in [9] was spatially periodic. Accordingly, comparison with [9] can be only qualitative.}\]
the $z$-direction) is significantly larger in the case of the Winckelmans–Leonard kernel than that with the Rosenhead–Moore kernel. It suggests that the complex three-dimensional evolution of vorticity at finite resolution is sensitive to the choice of a specific desingularization technique, while more symmetric flow configurations may obscure the difference.

When the numerical parameters are kept the same, it turns out that two kernels maintain a similar number of elements. For instance, at $t = 5$, the number of vortex elements in RM1 is 334,121, while the number in WL1 is 342,251. In theory, the refinement achieved by halving $\Delta x$ may lead to eight times more vortex elements, though the ratio in reality can be different from this estimate, depending on the numerical parameters specified for particle deletion after each iteration. In this particular case,
about two million vortex elements are used at $t = 5$ in RM2 and WL2, which results in the ratio roughly of 5.5. If we assume that the computational time consumed by the tree-code behaves as $O(N)$ and that the use of a Winckelmans–Leonard kernel doubles the computational time, WL1 should consume only 25% (from the estimate) and 36% (from the number ratio observed at $t = 5$) of the computational time compared to that used in RM2, for a single evaluation of the velocity field. If we count the smaller time step size used in the refined calculations, it becomes obvious that the overall computational saving achieved by the use of the Winckelmans–Leonard kernel is truly considerable.

4. Summary. A recurrence relation for the Taylor coefficients of the high-order algebraic kernel for vortex methods in three dimensions (the Winckelmans–Leonard kernel) is presented. An error estimate is obtained to ensure adaptive error control. The recurrence relation is integrated within a tree-code to evaluate vorticity-induced velocity. A numerical example shows that, relative to direct summation, the new tree-code for the Winckelmans–Leonard kernel provides accuracy and speed-up comparable to the tree-code for the Rosenhead–Moore kernel.

We then discuss the convergence characteristics of two algebraic kernels, i.e., the Rosenhead–Moore kernel and the Winckelmans–Leonard kernel. Both algebraic kernels lead to convergence in practice. For a typical resolution, the numerical error from the Winckelmans–Leonard kernel is an order of magnitude smaller than that from the Rosenhead–Moore kernel. As expected, the Winckelmans–Leonard kernel shows a superior convergence rate. Since the additional cost of using the Winckelmans–Leonard kernel instead of the Rosenhead–Moore kernel is minimal, it is recommended to use the Winckelmans–Leonard kernel for high-resolution vortex calculations.

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