Far-Field Evaluation to Compute the Linking Number with a Two-Tree Barnes–Hut

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This is a supplemental document for our paper, Fast Linking Numbers for Topology Verification of Loopy Structures.[2] This document should guide the reader in implementing the two-tree Barnes–Hut far-field evaluation for accumulating the linking number integral between two polylines.

1 Set up and notation

Here is the Barnes–Hut far-field expansion from our paper [2], expanded about $(\tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_2)$:

$$\lambda = -\int \mathrm{d}s\ \mathrm{d}t\ (\mathbf{r}_1' \times \mathbf{r}_2') \cdot \boldsymbol{\nabla} G(\mathbf{r}_1, \mathbf{r}_2). \tag{1}$$

$$\begin{aligned}\lambda = -\int \mathrm{d}s\ \mathrm{d}t\ \Big[&(\mathbf{r}_1' \times \mathbf{r}_2') \cdot \boldsymbol{\nabla} G(\tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_2)\\ &+ ((\mathbf{r}_1' \times \mathbf{r}_2') \otimes (-(\mathbf{r}_1 - \tilde{\mathbf{r}}_1) + (\mathbf{r}_2 - \tilde{\mathbf{r}}_2))) \cdot \boldsymbol{\nabla}^2 G(\tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_2)\\ &+ \frac{1}{2}((\mathbf{r}_1' \times \mathbf{r}_2') \otimes (-(\mathbf{r}_1 - \tilde{\mathbf{r}}_1) + (\mathbf{r}_2 - \tilde{\mathbf{r}}_2)) \otimes (-(\mathbf{r}_1 - \tilde{\mathbf{r}}_1) + (\mathbf{r}_2 - \tilde{\mathbf{r}}_2))) \cdot \boldsymbol{\nabla}^3 G(\tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_2)\\ &+ O(|\tilde{\mathbf{r}}_1 - \tilde{\mathbf{r}}_2|^{-5})\Big].\end{aligned} \tag{2}$$

Here the subscripts 1 and 2 refer to the two different curves, and ds and dt parameterize the curves, respectively, for the double line integral. That is, $\mathbf{r}_1 = \mathbf{r}_1(s)$, $\mathbf{r}_2 = \mathbf{r}_2(t)$, $\mathbf{r}_1' = \mathrm{d}\mathbf{r}_1/\mathrm{d}s$, and $\mathbf{r}_2' = \mathrm{d}\mathbf{r}_2/\mathrm{d}t$. We use Cartesian coordinates in this derivation and in our implementation.

Here are some helpful definitions. The $\otimes$ symbol denotes an outer product, and the dot product $(\cdot)$ denotes an inner product over all dimensions in order, e.g., if A and B are 2-tensors, then

$$A \cdot B = \sum_{i=1}^{3} \sum_{j=1}^{3} A_{ij} B_{ij}.$$

Furthermore, any two tensors written adjacent to each other indicates contracting the last index of the left tensor with the first index of the right tensor (e.g. matrix multiplication); for example, if A is a 2-tensor and B is a 3-tensor, then AB can be defined by

$$(AB)_{ijk} = \sum_{l=1}^{3} A_{il} B_{ljk}.$$

2 Derivatives of $G(\tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_2)$

Here are the derivatives of $G(\tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_2)$. Let $\tilde{\mathbf{r}} = \tilde{\mathbf{r}}_2 - \tilde{\mathbf{r}}_1$. Then

$$\nabla G(\tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_2) = \frac{\tilde{\mathbf{r}}}{4\pi|\tilde{\mathbf{r}}|^3}; \tag{3}$$

$$\nabla^2 G(\tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_2) = \frac{I_{3\times 3}|\tilde{\mathbf{r}}|^2 - 3\tilde{\mathbf{r}} \otimes \tilde{\mathbf{r}}}{4\pi|\tilde{\mathbf{r}}|^5}; \tag{4}$$

$$\nabla^3 G(\tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_2) = \frac{-3\sum_{i=1}^{3}(\tilde{\mathbf{r}} \otimes \mathbf{e}_i \otimes \mathbf{e}_i + \mathbf{e}_i \otimes \tilde{\mathbf{r}} \otimes \mathbf{e}_i + \mathbf{e}_i \otimes \mathbf{e}_i \otimes \tilde{\mathbf{r}})}{4\pi|\tilde{\mathbf{r}}|^5} + \frac{15\tilde{\mathbf{r}} \otimes \tilde{\mathbf{r}} \otimes \tilde{\mathbf{r}}}{4\pi|\tilde{\mathbf{r}}|^7}, \tag{5}$$

where $\mathbf{e}_i$ is the i-th basis element. Note that these are identical to the basis functions in Appendix A of [1], except the third derivative there (Eq. 24 in [1]) has a misprint.

These expressions can be expanded and rearranged so that for each term, the s and t integrals can be separated; this allows us to use the multipole moments directly.

3 Computing the Multipole Moment Tree

Let's discuss how to build the moment tree. Here are the moments:

$$\mathbf{c}_M = \int \mathbf{r}' \, \mathrm{d}s; \tag{6}$$

$$C_D = \int \mathbf{r}'(\mathbf{r} - \tilde{\mathbf{r}})^T \, \mathrm{d}s; \tag{7}$$

$$C_Q = \int \mathbf{r}' \otimes (\mathbf{r} - \tilde{\mathbf{r}}) \otimes (\mathbf{r} - \tilde{\mathbf{r}}) \, \mathrm{d}s. \tag{8}$$

For a line-segment element, we set $\tilde{\mathbf{r}}$ to the midpoint, and, evaluating the integrals over a line segment, we get that $\mathbf{c}_M$ is the displacement between the endpoints, $C_D = 0$, and $C_Q = \frac{1}{12}\mathbf{c}_M \otimes \mathbf{c}_M \otimes \mathbf{c}_M$.

When we combine bounding boxes into their parents, we need to sum and shift moments. We append the subscript p or c to $\mathbf{c}_M$, C_D, C_Q to denote whether it's the moment for the parent or child node, respectively. Let $\mathbf{r}_c$ be the displacement $\tilde{\mathbf{r}}_c - \tilde{\mathbf{r}}_p$ (from the parent node, indexed by p, to the child node, c), and simply use

$$\mathbf{c}_{Mp} = \sum_c \mathbf{c}_{Mc}; \tag{9}$$

$$C_{Dp} = \sum_c C_{Dc} + \mathbf{c}_{Mc}\mathbf{r}_c^T; \tag{10}$$

$$C_{Qpijk} = \sum_c C_{Qcijk} + C_{Dcij}r_{ck} + C_{Dcik}r_{cj} + c_{Mci}r_{cj}r_{ck}, \tag{11}$$

to compute the parent moments ($\mathbf{c}_{Mp}$, C_{Dp}, and C_{Qp}).

4 Evaluating a Far-Field Expansion Using Moments Between Two Nodes at $\tilde{\mathbf{r}}_1$ and $\tilde{\mathbf{r}}_2$

We can now rewrite the Barnes–Hut far-field expansion (Eq. (2)) using the moments we just built. The final results in §4.4 are what we use in our implementation.

Append the subscript 1 or 2 to $\mathbf{c}_M$, C_D, C_Q to denote whether it's the moment for the node at $\tilde{\mathbf{r}}_1$ or $\tilde{\mathbf{r}}_2$, respectively. Furthermore, let $\mathbf{p}_1 = \mathbf{r}_1 - \tilde{\mathbf{r}}_1$, $\mathbf{p}_2 = \mathbf{r}_2 - \tilde{\mathbf{r}}_2$. We will look at the different orders of the Barnes–Hut far-field expansion separately: the monopole term t_M (which contains ∇G), the dipole term t_D (which contains $\nabla^2 G$), and the quadrupole term t_Q (which contains $\nabla^3 G$). The dipole implementation on the GPU uses $\tilde{\lambda} = t_M + t_D$, and the quadrupole implementation on the CPU uses $\tilde{\lambda} = t_M + t_D + t_Q$, to approximate the linking integral over these two nodes.

4.1 Monopole:

Let's call the monopole term (which contains $\boldsymbol{\nabla} G$ in the integrand) t_M.

$$\begin{aligned} t_M &= -\int \mathrm{d}s\,\mathrm{d}t\,(\mathbf{r}_1' \times \mathbf{r}_2') \cdot \boldsymbol{\nabla} G, \\ &= \frac{-1}{4\pi|\tilde{\mathbf{r}}|^3} \left(\int \mathrm{d}s\,\mathbf{r}_1'\right) \times \left(\int \mathrm{d}t\,\mathbf{r}_2'\right) \cdot \tilde{\mathbf{r}}, \\ &= \frac{-1}{4\pi|\tilde{\mathbf{r}}|^3} \tilde{\mathbf{r}} \cdot (\mathbf{c}_{M1} \times \mathbf{c}_{M2}). \end{aligned} \tag{12}$$

4.2 Dipole:

Let's call the dipole terms (which contain $\boldsymbol{\nabla}^2 G$ in the integrand) t_D.

$$t_D = -\int \mathrm{d}s\,\mathrm{d}t\,((\mathbf{r}_1' \times \mathbf{r}_2') \otimes (-\mathbf{p}_1 + \mathbf{p}_2)) \cdot \boldsymbol{\nabla}^2 G; \tag{13}$$

$$4\pi|\tilde{\mathbf{r}}|^5 \boldsymbol{\nabla}^2 G = |\tilde{\mathbf{r}}|^2 I_{3\times 3} - 3\tilde{\mathbf{r}} \otimes \tilde{\mathbf{r}}. \tag{14}$$

Let t_{Da} be the contribution from the first term in the RHS of (14), and t_{Db} be the contribution from the second term. Then $t_D = t_{Da} + t_{Db}$.

$$\begin{aligned} t_{Da} &= \frac{-1}{4\pi|\tilde{\mathbf{r}}|^3} \int \mathrm{d}s\,\mathrm{d}t\,((\mathbf{r}_1' \times \mathbf{r}_2') \otimes (-\mathbf{p}_1 + \mathbf{p}_2)) \cdot I_{3\times 3}, \\ &= \frac{-1}{4\pi|\tilde{\mathbf{r}}|^3} \int \mathrm{d}s\,\mathrm{d}t\,((\mathbf{r}_1' \times \mathbf{r}_2') \cdot (-\mathbf{p}_1 + \mathbf{p}_2)), \\ &= \frac{-1}{4\pi|\tilde{\mathbf{r}}|^3} \left(\left(\int \mathrm{d}s\,(\mathbf{r}_1' \times \mathbf{p}_1)\right) \cdot \left(\int \mathrm{d}t\,\mathbf{r}_2'\right) + \left(\int \mathrm{d}t\,(\mathbf{r}_2' \times \mathbf{p}_2)\right) \cdot \left(\int \mathrm{d}s\,\mathbf{r}_1'\right) \right), \\ &= \frac{-1}{4\pi|\tilde{\mathbf{r}}|^3} \epsilon_{ijk} (C_{D1ij} c_{M2k} + C_{D2ij} c_{M1k}), \end{aligned} \tag{15}$$

where ϵ_{ijk} is the Levi-Cevita symbol, and terms with repeated indices ($\{i, j, k, l, m\}$) are summed across the three dimensions $(1, 2, 3)$ for each index (Einstein notation).

$$\begin{aligned} t_{Db} &= \frac{+3}{4\pi|\tilde{\mathbf{r}}|^5} \int \mathrm{d}s\,\mathrm{d}t\,((\mathbf{r}_1' \times \mathbf{r}_2') \otimes (-\mathbf{p}_1 + \mathbf{p}_2)) \cdot (\tilde{\mathbf{r}} \otimes \tilde{\mathbf{r}}), \\ &= \frac{+3}{4\pi|\tilde{\mathbf{r}}|^5} \int \mathrm{d}s\,\mathrm{d}t\,(((\mathbf{r}_1' \times \mathbf{r}_2') \cdot \tilde{\mathbf{r}})((-\mathbf{p}_1 + \mathbf{p}_2) \cdot \tilde{\mathbf{r}})), \\ &= \frac{-3}{4\pi|\tilde{\mathbf{r}}|^5} \int \mathrm{d}s\,\mathrm{d}t\,((\tilde{\mathbf{r}} \cdot \mathbf{p}_1)(\mathbf{r}_1' \cdot (\mathbf{r}_2' \times \tilde{\mathbf{r}})) + (\tilde{\mathbf{r}} \cdot \mathbf{p}_2)(\mathbf{r}_2' \cdot (\mathbf{r}_1' \times \tilde{\mathbf{r}}))), \\ &= \frac{-3}{4\pi|\tilde{\mathbf{r}}|^5} \left(\tilde{\mathbf{r}}^T \left(\int \mathrm{d}s\,\mathbf{p}_1 \mathbf{r}_1'^T\right) \left(\left(\int \mathrm{d}t\,\mathbf{r}_2'\right) \times \tilde{\mathbf{r}} \right) + \tilde{\mathbf{r}}^T \left(\int \mathrm{d}t\,\mathbf{p}_2 \mathbf{r}_2'^T\right) \left(\left(\int \mathrm{d}s\,\mathbf{r}_1'\right) \times \tilde{\mathbf{r}} \right) \right), \\ &= \frac{-3}{4\pi|\tilde{\mathbf{r}}|^5} ((C_{D1}\tilde{\mathbf{r}}) \cdot (\mathbf{c}_{M2} \times \tilde{\mathbf{r}}) + (C_{D2}\tilde{\mathbf{r}}) \cdot (\mathbf{c}_{M1} \times \tilde{\mathbf{r}})). \end{aligned} \tag{16}$$

Therefore

$$t_D = \frac{-1}{4\pi|\tilde{\mathbf{r}}|^5} (|\tilde{\mathbf{r}}|^2 \epsilon_{ijk} (C_{D1ij} c_{M2k} + C_{D2ij} c_{M1k}) + 3((C_{D1}\tilde{\mathbf{r}}) \cdot (\mathbf{c}_{M2} \times \tilde{\mathbf{r}}) + (C_{D2}\tilde{\mathbf{r}}) \cdot (\mathbf{c}_{M1} \times \tilde{\mathbf{r}}))). \tag{17}$$

4.3 Quadrupole:

Let's call the quadrupole terms (which contain $\boldsymbol{\nabla}^3 G$ in the integrand) t_Q, and index any subterms by t_{Qa}, t_{Qb}, t_{Qc}, and t_{Qd}, such that they sum to t_Q.

Let's first expand the $(-\mathbf{p}_1+\mathbf{p}_2)\otimes(-\mathbf{p}_1+\mathbf{p}_2)$ in t_Q:

$$t_Q = -\frac{1}{2}\int \mathrm{d}s\,\mathrm{d}t\,((\mathbf{r}_1'\times\mathbf{r}_2')\otimes(-\mathbf{p}_1+\mathbf{p}_2)\otimes(-\mathbf{p}_1+\mathbf{p}_2))\cdot\boldsymbol{\nabla}^3 G. \tag{18}$$

$$t_{Qa} = -\frac{1}{2}\int \mathrm{d}s\,\mathrm{d}t\,((\mathbf{r}_1'\times\mathbf{r}_2')\otimes\mathbf{p}_1\otimes\mathbf{p}_1)\cdot\boldsymbol{\nabla}^3 G, \tag{19}$$

$$t_{Qb} = \frac{1}{2}\int \mathrm{d}s\,\mathrm{d}t\,((\mathbf{r}_1'\times\mathbf{r}_2')\otimes\mathbf{p}_1\otimes\mathbf{p}_2)\cdot\boldsymbol{\nabla}^3 G, \tag{20}$$

$$t_{Qc} = \frac{1}{2}\int \mathrm{d}s\,\mathrm{d}t\,((\mathbf{r}_1'\times\mathbf{r}_2')\otimes\mathbf{p}_2\otimes\mathbf{p}_1)\cdot\boldsymbol{\nabla}^3 G, \text{ and} \tag{21}$$

$$t_{Qd} = -\frac{1}{2}\int \mathrm{d}s\,\mathrm{d}t\,((\mathbf{r}_1'\times\mathbf{r}_2')\otimes\mathbf{p}_2\otimes\mathbf{p}_2)\cdot\boldsymbol{\nabla}^3 G. \tag{22}$$

In Einstein notation,

$$(\boldsymbol{\nabla}^3 G)_{ijk} = \frac{3}{4\pi|\tilde{\mathbf{r}}|^7}(5\tilde{r}_i\tilde{r}_j\tilde{r}_k - |\tilde{\mathbf{r}}|^2(\tilde{r}_i\delta_{jk}+\tilde{r}_j\delta_{ik}+\tilde{r}_k\delta_{ij})). \tag{23}$$

where δ_{ij} is the identity matrix $I_{3\times3}$.

Let's simplify t_{Qa}. Also note that C_Q is symmetric in its last two dimensions.

$$\begin{aligned}
t_{Qa} &= -\frac{1}{2}\int \mathrm{d}s\,\mathrm{d}t\,((\mathbf{r}_1'\times\mathbf{r}_2')\otimes\mathbf{p}_1\otimes\mathbf{p}_1)\cdot\boldsymbol{\nabla}^3 G,\\
&= \frac{1}{2}\left(\left(\int \mathrm{d}t\,[\mathbf{r}_2']_\times\right)\left(\int \mathrm{d}s\,\mathbf{r}_1'\otimes\mathbf{p}_1\otimes\mathbf{p}_1\right)\right)\cdot\boldsymbol{\nabla}^3 G,\\
&= \frac{1}{2}\epsilon_{ijk}c_{M2i}C_{Q1jlm}(\boldsymbol{\nabla}^3 G)_{klm},\\
&= \frac{3\epsilon_{ijk}}{8\pi|\tilde{\mathbf{r}}|^7}\left(5c_{M2i}C_{Q1jlm}\tilde{r}_k\tilde{r}_l\tilde{r}_m - |\tilde{\mathbf{r}}|^2(c_{M2i}C_{Q1jll}\tilde{r}_k + 2c_{M2i}C_{Q1jkl}\tilde{r}_l)\right).
\end{aligned} \tag{24}$$

Similarly, let's simplify t_{Qb}:

$$\begin{aligned}
t_{Qb} &= \frac{1}{2}\int \mathrm{d}s\,\mathrm{d}t\,((\mathbf{r}_1'\times\mathbf{r}_2')\otimes\mathbf{p}_1\otimes\mathbf{p}_2)\cdot\boldsymbol{\nabla}^3 G,\\
&= \frac{1}{2}\epsilon_{ijk}C_{D1il}C_{D2jm}(\boldsymbol{\nabla}^3 G)_{klm},\\
&= \frac{3\epsilon_{ijk}}{8\pi|\tilde{\mathbf{r}}|^7}\left(5C_{D1il}C_{D2jm}\tilde{r}_k\tilde{r}_l\tilde{r}_m + |\tilde{\mathbf{r}}|^2(C_{D1ij}C_{D2kl}\tilde{r}_l - C_{D1il}C_{D2jk}\tilde{r}_l - C_{D1il}C_{D2jl}\tilde{r}_k)\right).
\end{aligned} \tag{25}$$

Because $\boldsymbol{\nabla}^3 G$ is symmetric in its last two dimensions, $t_{Qc} = t_{Qb}$.

By symmetry to t_{Qa},

$$t_{Qd} = \frac{-3\epsilon_{ijk}}{8\pi|\tilde{\mathbf{r}}|^7}\left(5c_{M1i}C_{Q2jlm}\tilde{r}_k\tilde{r}_l\tilde{r}_m - |\tilde{\mathbf{r}}|^2(c_{M1i}C_{Q2jll}\tilde{r}_k + 2c_{M1i}C_{Q2jkl}\tilde{r}_l)\right). \tag{26}$$

Summing and sanitizing each term by rearranging indices alphabetically,

$$\begin{aligned}
t_Q = \frac{3\epsilon_{ijk}}{8\pi|\tilde{\mathbf{r}}|^7}\big(&5\tilde{r}_i\tilde{r}_l\tilde{r}_m(c_{M2j}C_{Q1klm} - c_{M1j}C_{Q2klm} + 2C_{D1jl}C_{D2km})\\
&+ |\tilde{\mathbf{r}}|^2\tilde{r}_i(c_{M1j}C_{Q2kll} - c_{M2j}C_{Q1kll} - 2C_{D1jl}C_{D2kl})\\
&+ 2|\tilde{\mathbf{r}}|^2\tilde{r}_l(c_{M1i}C_{Q2jkl} - c_{M2i}C_{Q1jkl} + C_{D1ij}C_{D2kl} - C_{D1il}C_{D2jk})\big).
\end{aligned} \tag{27}$$

4.4 The Three Terms:

Putting them together:

$$t_M = \frac{-1}{4\pi|\tilde{\mathbf{r}}|^3}\tilde{\mathbf{r}} \cdot (\mathbf{c}_{M1} \times \mathbf{c}_{M2}); \tag{28}$$

$$t_D = \frac{-1}{4\pi|\tilde{\mathbf{r}}|^5}(|\tilde{\mathbf{r}}|^2\epsilon_{ijk}(C_{D1ij}c_{M2k} + C_{D2ij}c_{M1k}) + 3((C_{D1}\tilde{\mathbf{r}}) \cdot (\mathbf{c}_{M2} \times \tilde{\mathbf{r}}) + (C_{D2}\tilde{\mathbf{r}}) \cdot (\mathbf{c}_{M1} \times \tilde{\mathbf{r}}))); \tag{29}$$

$$\begin{aligned} t_Q = \frac{3\epsilon_{ijk}}{8\pi|\tilde{\mathbf{r}}|^7} \big(&5\tilde{r}_i\tilde{r}_l\tilde{r}_m(c_{M2j}C_{Q1klm} - c_{M1j}C_{Q2klm} + 2C_{D1jl}C_{D2km}) \\ &+ |\tilde{\mathbf{r}}|^2\tilde{r}_i(c_{M1j}C_{Q2kll} - c_{M2j}C_{Q1kll} - 2C_{D1jl}C_{D2kl}) \\ &+ 2|\tilde{\mathbf{r}}|^2\tilde{r}_l(c_{M1i}C_{Q2jkl} - c_{M2i}C_{Q1jkl} + C_{D1ij}C_{D2kl} - C_{D1il}C_{D2jk})\big) . \end{aligned} \tag{30}$$

As stated earlier, we use the dipole approximation, $\tilde{\lambda} = t_M + t_D$, on the GPU, and the quadrupole approximation, $\tilde{\lambda} = t_M + t_D + t_Q$, on the CPU, to compute the contribution to the Gauss linking integral from a pair of nodes.

References

[1] Gavin Barill, Neil G. Dickson, Ryan Schmidt, David I. W. Levin, and Alec Jacobson. Fast winding numbers for soups and clouds. *ACM Transactions on Graphics (TOG)*, 37(4):43:1–43:12, August 2018.

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