

One Term Real Sums

The one term, real sum part of the Ewald summation is presented here. Formulas are presented for corrections to the velocity, velocity gradient, velocity Laplacian and gradient of the velocity Laplacian. The fluid velocity at the center of any particle (or at any other point in the fluid) can be calculated analytically by simply adding the contributions given below for all neighboring particles. It is again noted that a self term (corresponding to $\mathbf{x} = 0$ must always be added when the fluid velocity is calculated at a center of a particle.

1. Force: F_i

The j -component of the net force F_j acting at a particles center, generates a disturbance velocity (velocity gradient and higher derivatives of the velocity) and disturbance pressure in the fluid, given by:

Velocity

for $\mathbf{x} \neq 0$:

$$u_i = -\frac{1}{4\pi\eta} \left[-\phi_{\frac{1}{2}} \left(\frac{\pi}{\alpha^{\frac{3}{2}}} \right) r^2 \delta_{ij} + \alpha^{-\frac{1}{2}} \phi_{-\frac{1}{2}} \delta_{ij} + \pi \alpha^{-\frac{3}{2}} \phi_{\frac{1}{2}} x_i x_j \right] F_j, \quad (1.1)$$

and for $\mathbf{x} = 0$:

$$u_i = -\frac{1}{4\pi\eta} \left(-\frac{2}{\alpha^{\frac{1}{2}}} \right) F_i. \quad (1.2)$$

(Note: F_i corresponds to the hydrodynamic force on the particle; the hydrodynamic force on the fluid has the opposite sign.)

Velocity Gradient

for $\mathbf{x} \neq 0$:

$$\frac{\partial u_i}{\partial x_k} = -\frac{1}{4\pi\eta} \left[-\frac{\pi}{\alpha^{\frac{3}{2}}} \left(4\delta_{ij} x_k - \delta_{jk} x_i - \delta_{ik} x_j \right) \phi_{\frac{1}{2}} + \frac{2\pi^2}{\alpha^{\frac{5}{2}}} \left(r^2 \delta_{ij} x_k - x_i x_j x_k \right) \phi_{\frac{3}{2}} \right] F_j, \quad (1.3)$$

and for $\mathbf{x} = 0$:

$$\frac{\partial u_i}{\partial x_k} = 0. \quad (1.4)$$

Velocity Laplacian

for $\mathbf{x} \neq 0$:

$$\begin{aligned} \nabla^2 u_i = & -\frac{1}{4\pi\eta} \left[-\frac{4\pi^3}{\alpha^{\frac{7}{2}}} \left(r^4 \delta_{ij} - r^2 x_i x_j \right) \phi_{\frac{5}{2}} + \frac{2\pi^2}{\alpha^{\frac{5}{2}}} \left(9r^2 \delta_{ij} - 7x_i x_j \right) \phi_{\frac{3}{2}} \right. \\ & \left. - \frac{10\pi}{\alpha^{\frac{3}{2}}} \delta_{ij} \phi_{\frac{1}{2}} \right] F_j, \end{aligned} \quad (1.5)$$

and for $\mathbf{x} = 0$:

$$\nabla^2 u_i = -\frac{1}{4\pi\eta} \left(\frac{20}{3} \frac{\pi}{\alpha^{\frac{3}{2}}} \right) F_i. \quad (1.6)$$

Gradient of Velocity Laplacian

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for $\mathbf{x} \neq 0$:

$$\begin{aligned} \frac{\partial \nabla^2 u_i}{\partial x_l} = & -\frac{1}{4\pi\eta} \left[\frac{8\pi^4}{\alpha^{\frac{9}{2}}} \left(r^4 x_l \delta_{ij} - r^2 x_i x_j x_l \right) \phi_{\frac{7}{2}} \right. \\ & - \frac{4\pi^3}{\alpha^{\frac{7}{2}}} \left(13r^2 x_l \delta_{ij} - 9x_i x_j x_l - r^2 \delta_{il} x_j - r^2 \delta_{jl} x_i \right) \phi_{\frac{5}{2}} \\ & \left. + \frac{2\pi^2}{\alpha^{\frac{5}{2}}} \left(28\delta_{ij} x_l - 7\delta_{il} x_j - 7\delta_{jl} x_i \right) \phi_{\frac{3}{2}} \right] F_j, \end{aligned} \quad (1.7)$$

and for $\mathbf{x} = 0$:

$$\frac{\partial \nabla^2 u_i}{\partial x_l} = 0. \quad (1.8)$$

Pressure

$$P = -\frac{1}{4\pi\eta} \left[-\frac{2\pi^2}{\alpha^{\frac{5}{2}}} r^2 \phi_{\frac{3}{2}} + \frac{5\pi}{\alpha^{\frac{3}{2}}} \phi_{\frac{1}{2}} \right] x_j F_j. \quad (1.9)$$

2. First Force Moment: Dipole D_{ij}

The ij -component of the first force moment tensor, corresponding to the particle stresslet and torque produce a disturbance in the fluid velocity and pressure given by:

Velocity

for $\mathbf{x} \neq 0$:

$$u_i = -\frac{1}{4\pi\eta} \left[-\frac{\pi}{\alpha^{\frac{3}{2}}} \left(4\delta_{ij} x_k - \delta_{jk} x_i - \delta_{ik} x_j \right) \phi_{\frac{1}{2}} + \frac{2\pi^2}{\alpha^{\frac{5}{2}}} \left(r^2 \delta_{ij} x_k - x_i x_j x_k \right) \phi_{\frac{3}{2}} \right] D_{jk}, \quad (2.1)$$

and for $\mathbf{x} = 0$:

$$u_i = 0. \quad (2.2)$$

Velocity Gradient

for $\mathbf{x} \neq 0$:

$$\begin{aligned} \frac{\partial u_i}{\partial x_l} = & -\frac{1}{4\pi\eta} \left[-\frac{4\pi^3}{\alpha^{\frac{7}{2}}} \left(r^2 \delta_{ij} x_k x_l - x_i x_j x_k x_l \right) \phi_{\frac{5}{2}} \right. \\ & + \frac{2\pi^2}{\alpha^{\frac{5}{2}}} \left(6\delta_{ij} x_l x_k + r^2 \delta_{ij} \delta_{kl} - \delta_{jk} x_i x_l - \delta_{ik} x_l x_j - \delta_{il} x_j x_k - \delta_{jl} x_i x_k - \delta_{kl} x_i x_j \right) \phi_{\frac{3}{2}} \\ & \left. - \frac{\pi}{\alpha^{\frac{3}{2}}} \left(4\delta_{ij} \delta_{kl} - \delta_{jk} \delta_{il} - \delta_{ik} \delta_{jl} \right) \phi_{\frac{1}{2}} \right] D_{jk}, \end{aligned} \quad (2.3)$$

and for $\mathbf{x} = 0$:

$$\frac{\partial u_i}{\partial x_l} = -\frac{1}{4\pi\eta} \frac{2\pi}{3\alpha^{\frac{3}{2}}} \left(4D_{il} - D_{li} - \delta_{il} D_{jj} \right). \quad (2.4)$$

Velocity Laplacian

for $\mathbf{x} \neq 0$:

$$\nabla^2 u_i(\mathbf{x}) = -\frac{1}{4\pi\eta} \left[\frac{8\pi^4}{\alpha^{\frac{9}{2}}} \left(r^4 x_k \delta_{ij} - r^2 x_i x_j x_k \right) \phi_{\frac{7}{2}} \right.$$

$$\begin{aligned}
& -\frac{4\pi^3}{\alpha^{\frac{7}{2}}}\left(13r^2x_k\delta_{ij}-9x_ix_jx_k-r^2\delta_{ik}x_j-r^2\delta_{jk}x_i\right)\phi_{\frac{5}{2}} \\
& +\frac{2\pi^2}{\alpha^{\frac{5}{2}}}\left(28\delta_{ij}x_k-7\delta_{ik}x_j-7\delta_{jk}x_i\right)\phi_{\frac{3}{2}}\Big]D_{jk},
\end{aligned} \tag{2.5}$$

and for $\mathbf{x} = 0$:

$$\nabla^2 u_i = 0. \tag{2.6}$$

Gradient of Velocity Laplacian

for $\mathbf{x} \neq 0$:

$$\begin{aligned}
\frac{\partial \nabla^2 u_i}{\partial x_l} = & -\frac{1}{4\pi\eta}\left[-\frac{16\pi^5}{\alpha^{\frac{11}{2}}}\left(r^4\delta_{ij}x_kx_l-r^2x_ix_jx_kx_l\right)\phi_{\frac{9}{2}}\right. \\
& +\frac{8\pi^4}{\alpha^{\frac{9}{2}}}\left(17r^2\delta_{ij}x_lx_k-11x_ix_jx_lx_k+r^4\delta_{ij}\delta_{kl}-r^2\delta_{il}x_jx_k\right. \\
& \left.-r^2\delta_{jl}x_ix_k-r^2\delta_{kl}x_ix_j-r^2\delta_{jk}x_ix_l-r^2\delta_{ik}x_jx_l\right)\phi_{\frac{7}{2}} \\
& \left.-\frac{4\pi^3}{\alpha^{\frac{7}{2}}}\left(54\delta_{ij}x_kx_l+13r^2\delta_{ij}\delta_{kl}-r^2\delta_{jk}\delta_{il}-r^2\delta_{ik}\delta_{jl}\right.\right. \\
& \left.-9\delta_{il}x_jx_k-9\delta_{jl}x_ix_k-9\delta_{kl}x_ix_j-9\delta_{jk}x_ix_l-9\delta_{ik}x_jx_l\right)\phi_{\frac{5}{2}} \\
& \left.+\frac{2\pi^2}{\alpha^{\frac{5}{2}}}\left(28\delta_{ij}\delta_{kl}-7\delta_{ik}\delta_{jl}-7\delta_{jk}\delta_{il}\right)\phi_{\frac{3}{2}}\right]D_{jk},
\end{aligned} \tag{2.7}$$

and for $\mathbf{x} = 0$:

$$\frac{\partial \nabla^2 u_i}{\partial x_l} = -\frac{1}{4\pi\eta}\left[-\frac{28}{5}\frac{\pi^2}{\alpha^{\frac{5}{2}}}\left(4D_{il}-D_{li}-\delta_{il}D_{jj}\right)\right]. \tag{2.8}$$

Pressure

$$P = -\frac{1}{4\pi\eta}\left[\frac{2\pi^3}{\alpha^{\frac{7}{2}}}r^2x_jx_k\phi_{\frac{5}{2}}-\frac{2\pi^2}{\alpha^{\frac{5}{2}}}\left(r^2\delta_{jk}+7x_jx_k\right)\phi_{\frac{3}{2}}+\frac{5\pi}{\alpha^{\frac{3}{2}}}\delta_{jk}\phi_{\frac{1}{2}}\right]D_{jk}. \tag{2.9}$$

3. Second Force Moment: d_i

The i -component of the second force moment generates a velocity and pressure disturbance given by:

Velocity

for $\mathbf{x} \neq 0$:

$$\begin{aligned}
u_i = & -\frac{1}{4\pi\eta}\left[\frac{2\pi^3}{\alpha^{\frac{7}{2}}}\left(r^4\delta_{ij}-r^2x_ix_j\right)\phi_{\frac{5}{2}}\right. \\
& \left.-\frac{\pi^2}{\alpha^{\frac{5}{2}}}\left(9r^2\delta_{ij}-7x_ix_j\right)\phi_{\frac{3}{2}}\right. \\
& \left.+\frac{5\pi}{\alpha^{\frac{3}{2}}}\delta_{ij}\phi_{\frac{1}{2}}\right]d_j,
\end{aligned} \tag{3.1}$$

and for $\mathbf{x} = 0$:

$$\nabla^2 u_i = -\frac{1}{4\pi\eta} \left(-\frac{10}{3} \frac{\pi}{\alpha^{\frac{3}{2}}} \right) d_i. \quad (3.2)$$

Velocity gradient
for $\mathbf{x} \neq 0$:

$$\begin{aligned} \frac{\partial u_i}{\partial x_k} = & -\frac{1}{4\pi\eta} \left[-\frac{4\pi^4}{\alpha^{\frac{9}{2}}} \left(r^4 x_k \delta_{ij} - r^2 x_i x_j x_k \right) \phi_{\frac{7}{2}} \right. \\ & + \frac{2\pi^3}{\alpha^{\frac{7}{2}}} \left(13r^2 x_k \delta_{ij} - 9x_i x_j x_k - r^2 \delta_{ik} x_j - r^2 \delta_{jk} x_i \right) \phi_{\frac{5}{2}} \\ & \left. - \frac{\pi^2}{\alpha^{\frac{5}{2}}} \left(28\delta_{ij} x_k - 7\delta_{ik} x_j - 7\delta_{jk} x_i \right) \phi_{\frac{3}{2}} \right] d_j, \end{aligned} \quad (3.3)$$

and for $\mathbf{x} = 0$:

$$\frac{\partial u_i}{\partial x_k} = 0. \quad (3.4)$$

Velocity Laplacian
for $\mathbf{x} \neq 0$:

$$\begin{aligned} \nabla^2 u_i = & -\frac{1}{4\pi\eta} \left[\frac{8\pi^5}{\alpha^{\frac{11}{2}}} \left(r^6 \delta_{ij} - r^4 x_i x_j \right) \phi_{\frac{9}{2}} \right. \\ & - \frac{4\pi^4}{\alpha^{\frac{9}{2}}} \left(20r^4 \delta_{ij} - 18r^2 x_i x_j \right) \phi_{\frac{7}{2}} \\ & + \frac{2\pi^3}{\alpha^{\frac{7}{2}}} \left(91r^2 \delta_{ij} - 63x_i x_j \right) \phi_{\frac{5}{2}} \\ & \left. - \frac{\pi^2}{\alpha^{\frac{5}{2}}} \left(70\delta_{ij} \right) \right] d_j, \end{aligned} \quad (3.5)$$

$$- \frac{\pi^2}{\alpha^{\frac{5}{2}}} \left(70\delta_{ij} \right) \Big] d_j, \quad (3.6)$$

and for $\mathbf{x} = 0$:

$$\nabla^2 u_i = -\frac{1}{4\pi\eta} \left(\frac{28\pi^2}{\alpha^{\frac{5}{2}}} d_i \right). \quad (3.7)$$

Gradient of Velocity Laplacian
for $\mathbf{x} \neq 0$:

$$\begin{aligned} \frac{\partial \nabla^2 u_i}{\partial x_l} = & -\frac{1}{4\pi\eta} \left[-\frac{16\pi^6}{\alpha^{\frac{13}{2}}} \left(r^6 \delta_{ij} x_l - r^4 x_l x_i x_j \right) \phi_{\frac{11}{2}} \right. \\ & + \frac{8\pi^5}{\alpha^{\frac{11}{2}}} \left(26r^4 \delta_{ij} x_l - 22r^2 x_i x_j x_l - r^4 \delta_{il} x_j - r^4 \delta_{jl} x_i \right) \phi_{\frac{9}{2}} \\ & - \frac{4\pi^4}{\alpha^{\frac{9}{2}}} \left(171r^2 \delta_{ij} x_l - 99x_i x_j x_l - 18r^2 \delta_{il} x_j - 18r^2 \delta_{jl} x_i \right) \phi_{\frac{7}{2}} \\ & \left. + \frac{2\pi^3}{\alpha^{\frac{7}{2}}} \left(252\delta_{ij} x_l - 63\delta_{il} x_j - 63\delta_{jl} x_i \right) \phi_{\frac{5}{2}} \right] d_j, \end{aligned} \quad (3.8)$$

and for $\mathbf{x} = 0$:

$$\frac{\partial \nabla^2 u_i}{\partial x_l} = 0. \quad (3.9)$$

Pressure

$$P = -\frac{1}{4\pi\eta} \left[\frac{4\pi^4}{\alpha^{\frac{9}{2}}} r^4 x_j \phi_{\frac{7}{2}} - \frac{2\pi^3}{\alpha^{\frac{7}{2}}} 14r^2 x_j \phi_{\frac{5}{2}} + \frac{35\pi^2}{\alpha^{\frac{5}{2}}} x_j \phi_{\frac{3}{2}} \right] d_j. \quad (3.10)$$

4. Third Force moment: S_{ij}

The ij -component of the third force moment generates a velocity and pressure disturbance in the fluid given by:

Velocity
for $\mathbf{x} \neq 0$:

$$\begin{aligned} u_i = & -\frac{1}{4\pi\eta} \left[\frac{8\pi^4}{\alpha^{\frac{9}{2}}} \left(r^4 x_k \delta_{ij} - r^2 x_i x_j x_k \right) \phi_{\frac{7}{2}} \right. \\ & - \frac{4\pi^3}{\alpha^{\frac{7}{2}}} \left(13r^2 x_k \delta_{ij} - 9x_i x_j x_k - r^2 \delta_{ik} x_j - r^2 \delta_{jk} x_i \right) \phi_{\frac{5}{2}} \\ & \left. + \frac{2\pi^2}{\alpha^{\frac{5}{2}}} \left(28\delta_{ij} x_k - 7\delta_{ik} x_j - 7\delta_{jk} x_i \right) \phi_{\frac{3}{2}} \right] S_{jk}, \end{aligned} \quad (4.1)$$

and for $\mathbf{x} = 0$:

$$u_i = 0. \quad (4.2)$$

Velocity gradient
for $\mathbf{x} \neq 0$:

$$\begin{aligned} \frac{\partial u_i}{\partial x_l} = & -\frac{1}{4\pi\eta} \left[-\frac{16\pi^5}{\alpha^{\frac{11}{2}}} \left(r^4 \delta_{ij} x_k x_l - r^2 x_i x_j x_k x_l \right) \phi_{\frac{9}{2}} \right. \\ & + \frac{8\pi^4}{\alpha^{\frac{9}{2}}} \left(17r^2 \delta_{ij} x_k x_l + r^4 \delta_{ij} \delta_{kl} - 11x_i x_j x_k x_l - r^2 \delta_{il} x_j x_k \right. \\ & \left. - r^2 \delta_{jl} x_i x_k - r^2 \delta_{kl} x_i x_j - r^2 \delta_{jk} x_i x_l - r^2 \delta_{ik} x_j x_l \right) \phi_{\frac{7}{2}} \\ & - \frac{4\pi^3}{\alpha^{\frac{7}{2}}} \left(54\delta_{ij} x_k x_l + 13r^2 \delta_{ij} \delta_{kl} - 9\delta_{jk} x_i x_l - 9\delta_{ik} x_j x_l \right. \\ & \left. - 9\delta_{il} x_j x_k - 9\delta_{jl} x_i x_k - 9\delta_{kl} x_i x_j - r^2 \delta_{jk} \delta_{il} - r^2 \delta_{ik} \delta_{jl} \right) \phi_{\frac{5}{2}} \\ & \left. + \frac{2\pi^2}{\alpha^{\frac{5}{2}}} \left(28\delta_{ij} \delta_{kl} - 7\delta_{ik} \delta_{jl} - 7\delta_{jk} \delta_{il} \right) \phi_{\frac{3}{2}} \right] S_{jk}, \end{aligned} \quad (4.3)$$

and for $\mathbf{x} = 0$:

$$\frac{\partial u_i}{\partial x_l} = -\frac{1}{4\pi\eta} \left[\frac{28\pi^2}{5\alpha^{\frac{5}{2}}} \left(4S_{il} - S_{li} - \delta_{il} S_{jj} \right) \right]. \quad (4.4)$$

Velocity Laplacian
for $\mathbf{x} \neq 0$:

$$\nabla^2 u_i = -\frac{1}{4\pi\eta} \left[\frac{32\pi^6}{\alpha^{\frac{13}{2}}} \left(r^6 \delta_{ij} x_k - r^4 x_i x_j x_k \right) \phi_{\frac{11}{2}} \right]$$

$$\begin{aligned}
& -\frac{16\pi^5}{\alpha^{\frac{9}{2}}}\left(26r^4\delta_{ij}x_k - 22r^2x_ix_jx_k - r^4\delta_{jk}x_i - r^4\delta_{ik}x_j\right)\phi_{\frac{9}{2}} \\
& +\frac{8\pi^4}{\alpha^{\frac{7}{2}}}\left(171r^2\delta_{ij}x_k - 99x_ix_jx_k - 18r^2\delta_{ik}x_j - 18r^2\delta_{jk}x_i\right)\phi_{\frac{7}{2}} \\
& -\frac{4\pi^3}{\alpha^{\frac{5}{2}}}\left(252\delta_{ij}x_k - 63\delta_{jk}x_i - 63\delta_{ik}x_j\right)\phi_{\frac{5}{2}}\Big]S_{jk}, \tag{4.5}
\end{aligned}$$

and for $\mathbf{x} = 0$:

$$\nabla^2 u_i = 0. \tag{4.6}$$

Gradient of Velocity Laplacian

for $\mathbf{x} \neq 0$:

$$\begin{aligned}
\frac{\partial u_i}{\partial x_l} = & -\frac{1}{4\pi\eta}\left[-\frac{64\pi^7}{\alpha^{\frac{15}{2}}}\left(r^6\delta_{ij}x_kx_l - r^4x_ix_jx_kx_l\right)\phi_{\frac{13}{2}}\right. \\
& +\frac{32\pi^6}{\alpha^{\frac{13}{2}}}\left(32r^4\delta_{ij}x_kx_l + r^6\delta_{ij}\delta_{kl} - 26r^2x_ix_jx_kx_l - r^4\delta_{il}x_jx_k\right. \\
& \left.- r^4\delta_{jl}x_ix_k - r^4\delta_{kl}x_ix_j - r^4\delta_{jk}x_ix_l - r^4\delta_{ik}x_jx_l\right)\phi_{\frac{11}{2}} \\
& -\frac{16\pi^5}{\alpha^{\frac{11}{2}}}\left(275r^2\delta_{ij}x_kx_l + 26r^4\delta_{ij}\delta_{kl} - 143x_ix_jx_kx_l - 22r^2\delta_{jk}x_ix_l\right. \\
& \left.- 22r^2\delta_{ik}x_jx_l - 22r^2\delta_{il}x_jx_k - 22r^2\delta_{jl}x_ix_k - 22r^2\delta_{kl}x_ix_j - r^4\delta_{jk}\delta_{il} - r^4\delta_{ik}\delta_{jl}\right)\phi_{\frac{9}{2}} \\
& +\frac{8\pi^4}{\alpha^{\frac{9}{2}}}\left(594\delta_{ij}x_kx_l + 171r^2\delta_{ij}\delta_{kl} - 99\delta_{il}x_jx_k - 99\delta_{jl}x_ix_k\right. \\
& \left.- 99\delta_{kl}x_ix_j - 99\delta_{ik}x_lx_j - 99\delta_{jk}x_lx_i - 18r^2\delta_{jl}\delta_{ik} - 18r^2\delta_{il}\delta_{jk}\right)\phi_{\frac{7}{2}} \\
& \left.-\frac{4\pi^3}{\alpha^{\frac{7}{2}}}\left(252\delta_{ij}\delta_{kl} - 63\delta_{jk}\delta_{il} - 63\delta_{ik}\delta_{jl}\right)\phi_{\frac{5}{2}}\right]S_{jk}, \tag{4.7}
\end{aligned}$$

and for $\mathbf{x} = 0$:

$$\frac{\partial \nabla^2 u_i}{\partial x_l} = -\frac{1}{4\pi\eta}\left[\frac{72\pi^3}{\alpha^{\frac{7}{2}}}\left(4S_{il} - S_{li} - \delta_{il}S_{jj}\right)\right]. \tag{4.8}$$

Pressure

$$\begin{aligned}
P = & -\frac{1}{4\pi\eta}\left[\frac{16\pi^5}{\alpha^{\frac{11}{2}}}r^4x_jx_k\phi_{\frac{9}{2}} - \frac{8\pi^4}{\alpha^{\frac{9}{2}}}\left(18r^2x_jx_k + r^4\delta_{jk}\right)\phi_{\frac{7}{2}}\right. \\
& \left.+\frac{4\pi^3}{\alpha^{\frac{7}{2}}}\left(14r^2\delta_{jk} + 63x_jx_k\right)\phi_{\frac{5}{2}} - \frac{70\pi^2}{\alpha^{\frac{5}{2}}}\delta_{jk}\phi_{\frac{3}{2}}\right]S_{jk}. \tag{4.9}
\end{aligned}$$