Cubic volume and Surface area Computation

Evgueni Tcherniaev

Geant4 development team

Computational methods

- GetCubicVolume() **and** GetSurfaceArea() **are the basic methods that are available in all Geant4 solids**
- **Traditionally the following two methods were used for the calculations:**
  - *Analytical expressions*
  - *The Monte Carlo (MC) method*

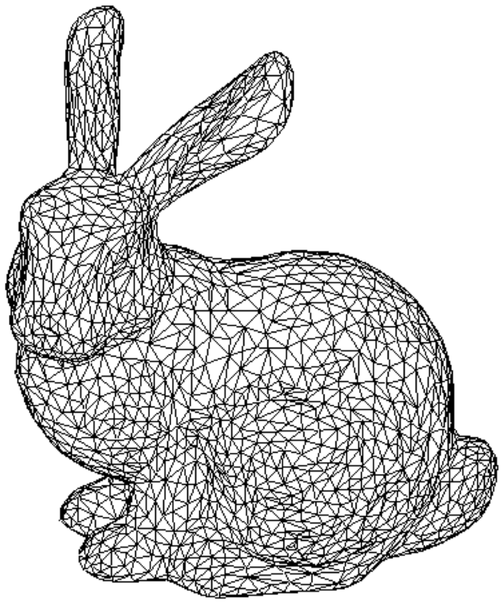
    GetCubicVolume() **and** GetSurfaceArea() **based on the MC method are implemented in the** G4VSolid **base class and can be called in all Geant4 solids as** G4VSolid::GetCubicVolume() **and** G4VSolid::GetCubicVolume()
- **There is yet another method –** ***numerical integration*****. It is faster and more precise than the MC method. First time it was applied in** Geant4 10.07 **for the computation of the Cubic volume and Surface area in** G4CutTubs**, and the Surface area in** G4Ellipsoid.

Geant4 Solids

- Solids bounded by planes
  G4Box, G4Para, G4Trd, G4Trap, G4Tet, G4Polyhedra, G4ExtrudedSolid, G4TessellatedSolid
  - no problem with analytical expressions
- Solids with curved surfaces
  a) G4Orb, G4Sphere, G4Tubs, G4Cons, G4Polycone, G4GenericPolycone, G4Torus
     - analytical expressions for these solids are well known or easy to derive
  b) G4CutTubs
     - special case
  c) G4EllipticalTube, G4EllipticalCone, G4Paraboloid, G4Hype, G4TwistedTube, G4TwistedBox, G4TwistedTrd
     - analytical expressions these solids are less known, or not so easy to derive on your own
  d) G4TwistedTrap, G4GenericTrap, G4Ellipsoid
     - no analytical expressions
- Composite solids
  Boolean solids: G4UnionSolid, G4SubtractionSolid, G4IntersectionSolid, G4MultiUnion;
  G4ScaledSolid, G4ReflectedSolid, G4DisplacedSolid
  - the MC method is used for the Boolean solids and for the computation of the surface are of G4ScaledSolid

Solids bounded by planes

Analytical expressions for computing the Cubic volume and Surface area for G4Box, G4Para, G4Trd, G4Trap, G4Tet, G4Polyhedra, G4ExtrudedSolid, G4TessellatedSolid are well known. The least obvious among these is the computing the Cubic volume for G4TesselatedSolid, the most general case of a solid bounded by planes:



$$V = \frac{1}{3}\left|\sum_{F}(P_F \cdot N_F)\,\mathrm{area}(F)\right|$$

where the sum is over faces F of the solid
P_F is a point on face F
N_F is a normal to F pointing outside of the solid
The dot (·) is the dot product

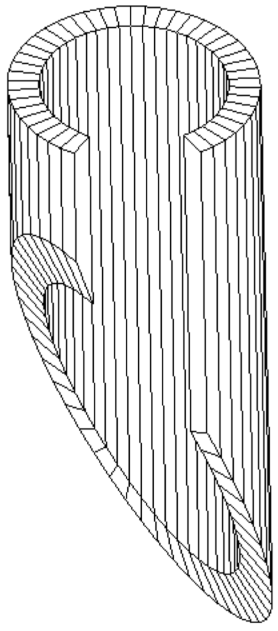
Composite solids

- These solids are compositions of one or two solids and a transformation:
  - Boolean solids: G4UnionSolid, G4SubtractionSolid, G4IntersectionSolid, G4MultiUnion
  - Transformed solids: G4ScaledSolid, G4ReflectedSolid, G4DisplacedSolid
- Boolean solids: computing the Cubic volume and Surface area is done by the MC method. An enhancement to the Cubic volume calculation in G4UnionSolid and G4SubtractionSolid, that improves the accuracy, has been implemented by John Apostolakis for Geant4 11.0
- The Cubic volume of G4ScaledSolid is computed by multiplying the Cubic Volume of the original solid by the scale factors. The Surface area is computed by the MC method
- G4ReflectedSolid, G4DisplacedSolid: reflection and Affine transformation do not change the Cubic volume and Surface area of the transformed solid

Solids with curved surfaces

- In general, finding analytical expressions for calculating the Cubic volume is not so difficult, and in the next slides I will mainly focus on the computing the Surface area.
- Relative to the computing the Surface area, the Geant4 solids with curved surfaces can be subdivided in four groups:
  a) G4Orb, G4Sphere, G4Tubs, G4Cons, G4Polycone, G4GenericPolycone, G4Torus - the analytical expressions are well known and will not be discussed
  b) G4CutTubs - special case
  c) G4EllipticalTube, G4EllipticalCone, G4Paraboloid, G4Hype, G4TwistedTube, G4TwistedBox, G4TwistedTrd - analytical expressions for these solids are less known, or not so easy to derive on your own
  d) G4TwistedTrap, G4GenericTrap, G4Ellipsoid - no analytical expressions

G4CutTubs(name, r_{min}, r_{max}, z, φ_0, $\Delta\varphi$, N_{low} , N_{high})



G4CutTubs is G4Tubs cut by two planes. If $\Delta\varphi = 2\pi$ then the computation of the Cubic volume and Surface area can be done analytically:

$$V = \pi h(r_{\max}^2 - r_{\max}^2)$$

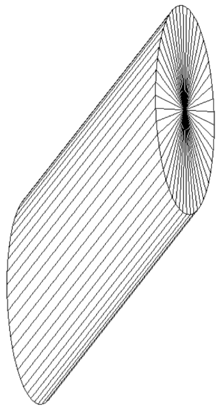
$$S = 2\pi h(r_{\max} - r_{\min}) + \pi(r_{\max}^2 - r_{\max}^2)\left(\frac{1}{|z_{\text{low}}|} + \frac{1}{|z_{\text{high}}|}\right)$$

$h = 2z$

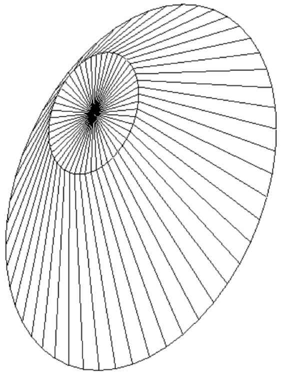
z_{low} , z_{high} – z-components of the normals

If $\Delta\varphi < 2\pi$ then the computing the Cubic volume and Surface area is done by numerical integration.

G4EllipticalTube(name, x, y, z)



G4EllipticalCone(name, x, y, z, zcut)



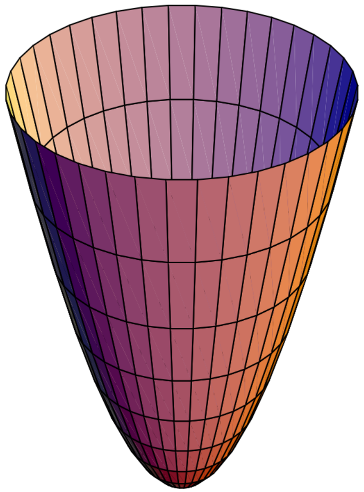
The analytical expressions for these solids are well known, but it worth noting that the calculation of the Surface area for these solids requires the use of a special function - *the complete elliptic integral of the second kind.* Such function was added in Geant4 10.04 as G4GeomTools::comp_ellint_2()

I did not check, but since C++ 17 the elliptic integrals should be a part of C+ math library, so G4GeomTools::comp_ellint_2() can be replaced with std::comp_ellint_2()

G4Paraboloid(name, z, r_1, r_2)

The computation of the Cubic volume and Surface area is based on the expressions for Paraboloid, see for example:

https://mathworld.wolfram.com/Paraboloid.html



$$V = \frac{1}{2}\pi a^2 h$$

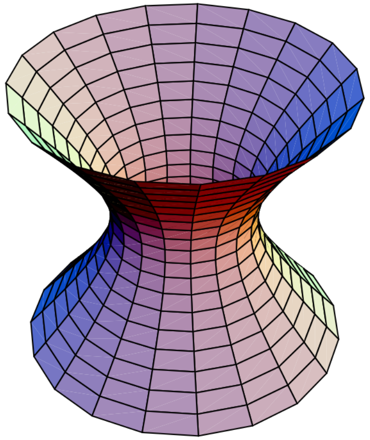
$$S = \frac{\pi a}{6h^2}\left[(a^2 + 4h^2)^{3/2} - a^3\right]$$

a – radius at the top cross section

G4Hype(name, r_{in}, r_{out}, $stereo_{in}$, $stereo_{out}$, z)

The computation of the Cubic volume and Surface area is based on the expressions for One-Sheeted Hyperboloid:

https://mathworld.wolfram.com/One-SheetedHyperboloid.html



Cartesian equation: $\frac{x^2}{a^2} + \frac{y^2}{a^2} - \frac{z^2}{c^2} = 1$

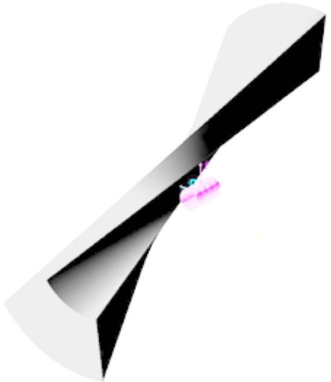
Volume: $V = \frac{1}{3}\pi h(2a^2 + R^2)$

Surface area: $S = 2\pi a \left[\frac{h\sqrt{\cancel{(a^2+c^2)}[4c^4+(a^2+c^2)h^2]}}{4c^2} + \frac{c^2 \sinh^{-1}\left(\frac{h\sqrt{a^2+c^2}}{2c^2}\right)}{\sqrt{a^2+c^2}} \right]$

radius at $z = 0$, h – full height, R – radius at the top cross section

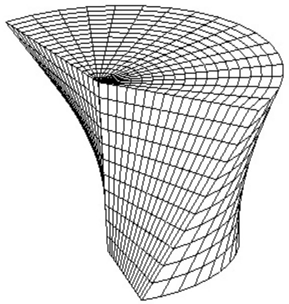
Note: There is a mistake in the expression for the Surface area (see crossed term), that is still present on the referred page despite being reported several months ago

All expressions for the Surface area on the next slides were obtained by myself. The expressions have been verified by comparison with the result of numerical integration.



G4TwistedTubs(name, ω, r_{in}, r_{out}, z_{neg}, z_{pos}, φ) *

For the reason that G4TwistedTubs may have bottom and top bases placed at different distance from the origin, the computation of the Cubic volume and Surface area is based on the expressions for a twisted half-cylinder segment



Volume of the half-cylinder segment: $V = \frac{\varphi h}{6}\,(2a^2 + r^2)$

- φ – size of the segment in radians
- h – height of the half-cylinder
- a – radius at $z = 0$
- r – radius at $z = h$

Lateral surface area: $S = \varphi a\left(h\sqrt{1 + k^2h^2} + \frac{1}{k}\sinh^{-1}(kh)\right)$

$$k = \frac{\sqrt{a^2 + c^2}}{c^2}, c^2 = \frac{a^2h^2}{r^2 - a^2}$$

Area of the face at the phi cut: $S = \frac{ah}{3pq}\left(pqf + \frac{p\left(p^3+3\right)}{2}\tanh^{-1}\left(\frac{q}{f}\right) + \frac{q\left(q^3+3\right)}{2}\tanh^{-1}\left(\frac{p}{f}\right) + \tan^{-1}\left(\frac{f}{pq}\right) - \frac{\pi}{2}\right)$

$p = \dfrac{r\sin\omega}{h}, q = \dfrac{r\sin\omega}{a}, f = \sqrt{p^2 + q^2 + 1}, \omega$ – twist angle

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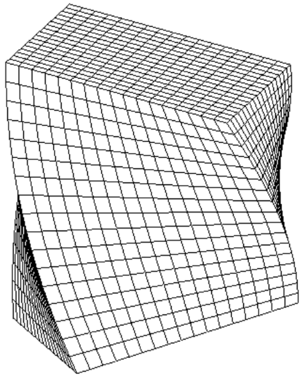
* The publication with the G4TwistedTubs implementation details: Kotoyo Hoshina, Keisuke Fujii, Osamu Nitoh, *Development of a Geant4 solid for stereo mini-jet cells in a cylindrical drift chamber*, Computer Physics Communications 153 (2003) pp.373–391

G4TwistedBox(name, ω, x, y, z)



Cubic volume: $V = 8xyz$

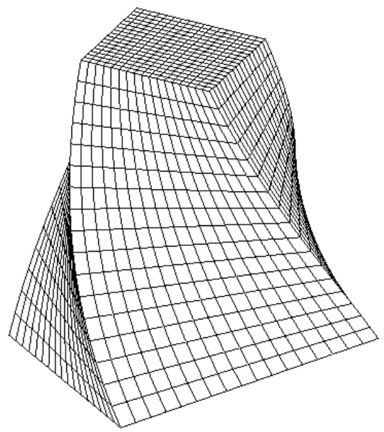
Surface area: $S = 2S_x + 2S_y + 8xy$

$$S_x = x\sqrt{h^2 + x^2\varphi^2} + \frac{h^2}{\varphi}\,\mathrm{asinh}\left(\frac{x\varphi}{h}\right)$$

where $h = 2z$ – full height, ω – twist angle

Expression for S_y is similar to the expression for S_x

G4TwistedTrd(name, x_1, x_2, y_1, y_2, z, ω)



Cubic volume: $V = 2(x_1 + x_2)(y_1 + y_2)z + \frac{2}{3}(x_2 - x_1)(y_2 - y_1)z$

Surface area: $S = 2S_x + 2S_y + 4(x_1 y_1 + x_2 y_2)$

$$S_x = \frac{(I_u + I_v)}{(x_2 - x_1)\omega^2}$$

$$I_u = \frac{1}{6}\left[(h^2 + (u_2)^2)^{\frac{3}{2}} - (h^2 + (u_1)^2)^{\frac{3}{2}}\right] + \frac{h^2}{2}\left[\left(u_2 \operatorname{asinh}\frac{u_2}{h} - u_1 \operatorname{asinh}\frac{u_1}{h}\right) - \left(\sqrt{h^2 + (u_2)^2} - \sqrt{h^2 + (u_1)^2}\right)\right]$$
$$I_v = \frac{1}{6}\left[(h^2 + (v_2)^2)^{\frac{3}{2}} - (h^2 + (v_1)^2)^{\frac{3}{2}}\right] + \frac{h^2}{2}\left[\left(v_2 \operatorname{asinh}\frac{v_2}{h} - v_1 \operatorname{asinh}\frac{v_1}{h}\right) - \left(\sqrt{h^2 + (v_2)^2} - \sqrt{h^2 + (v_1)^2}\right)\right]$$

$$u_1 = (y_2 - y_1) + x_1\omega, u_2 = (y_2 - y_1) + x_2\omega$$
$$v_1 = (y_2 - y_1) - x_1\omega, v_2 = (y_2 - y_1) - x_1\omega$$

Expression for S_y is similar to the expression for S_x

Fast numerical integration

- Very often a 3D surface can be represented in a parametric form:

$$\vec{r} = \vec{r}(s,t)$$

- The surface area can be computed with the following double integral:

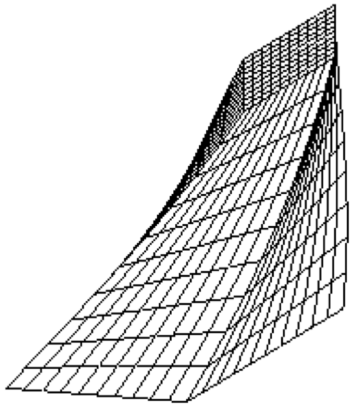
$$S = \int_{c}^{d}\int_{a}^{b} \left|\frac{\partial\vec{r}}{\partial s} \times \frac{\partial\vec{r}}{\partial t}\right| ds dt$$

- If the double integral cannot be found analytically, then we can evaluate it by numerical integration - the surface is divided into small quadrangles (e.g. 100x100) and the surface area is calculated as a sum of the areas of the quadrangles.
- We can try to also do something better – try to find an analytical expression for the inner integral, and then evaluate the outer integral numerically, the evaluation will be faster and more precise:

$$S = \int_{c}^{d} F(t) dt$$

- For comparison:
  - The MC method – 1 M random points, precision 10^{-2}
  - Ordinary numerical integration – 100x100 steps along two parameters, precision 10^{-4}
  - Fast numerical integration – 1000 steps along one parameter, precision 10^{-6}

G4TwistedTrap(name, ω, z, θ, φ, y_1, x_1, x_2, y_2, x_3, x_4, α)



Cubic volume: $V = (x_1 + x_2 + x_3 + x_4)(y_1 + y_2)z + \frac{1}{3}(x_4 + x_3 - x_2 - x_1)(y_2 - y_1)z$

Surface area:

$$S = \int_0^1 \left[\frac{2as+b}{4a}R + \frac{4ac-b^2}{8a}\frac{1}{\sqrt{a}}\ln\left|2\sqrt{a}\,R + 2as + b\right|\right]_{s=0}^{s=1} dt$$

$R = \sqrt{as^2 + bs + c}$

$a = A^2, b = 2AB, c = B^2 + h^2(I^2 + J^2)$

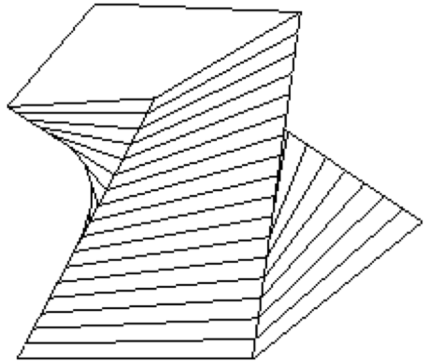
$A = \omega(I^2 + J^2) + (x_{21}y_{43} - x_{43}y_{21})$

$B = (Iy_{31} - Jx_{31}) + \omega I(x_1 + x_{31}t) + \omega J(y_1 + y_{31}t) + h\tan\theta\left[I\sin\left(\varphi + \frac{\omega}{2} - \omega t\right) - J\cos\left(\varphi + \frac{\omega}{2} - \omega t\right)\right]$

$I = x_{21} + (x_{43} - x_{21})t,\ J = y_{21} + (y_{43} - y_{21})t$

$x_{21} = x_2 - x_1, y_{21} = y_2 - y_1, x_{31} = x_3 - x_1, y_{31} = y_3 - y_1, x_{43} = x_4 - x_3, y_{43} = y_4 - y_3$

G4GenericTrap(name, z, v[8])



Cubic volume: $V = \frac{z}{3}(\mathbf{v}_{31}\times\mathbf{v}_{20} + \mathbf{v}_{75}\times\mathbf{v}_{64}) + \frac{z}{6}(\mathbf{v}_{31}\times\mathbf{v}_{64} + \mathbf{v}_{75}\times\mathbf{v}_{20})$

where $\mathbf{v}_{\mathrm{ik}} = \mathbf{v}_{\mathrm{i}} - \mathbf{v}_{\mathrm{k}}$, $\boldsymbol{a}\times\boldsymbol{b} = a_x b_y - a_y b_x$, z – half height

Surface area:

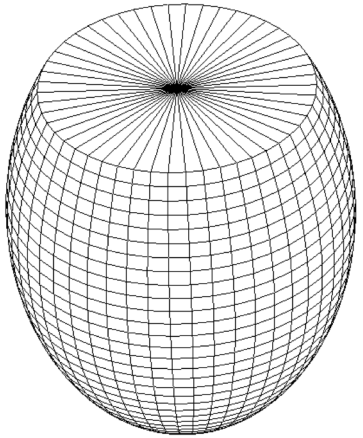
$$S = \int_0^1 \left[\frac{2as+b}{4a}R + \frac{4ac-b^2}{8a}\frac{1}{\sqrt{a}}\ln\left|2\sqrt{a}\,R + 2as + b\right|\right]_{s=0}^{s=1} dt$$

$R = \sqrt{as^2 + bs + c}$

$a = A^2, b = 2AB, c = I^2 + J^2 + B^2$

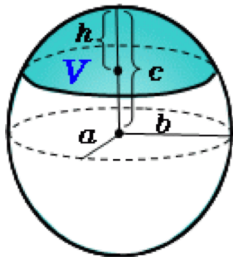
$A = (x_{21}y_{43} - y_{21}x_{43}), B = (y_{31}x_{42} - x_{31}y_{42})t + (x_{21}y_{31} - x_{31}y_{21})$

$I = (y_{43} - y_{21})ht + y_{21}h, J = (x_{43} - x_{21})ht + x_{21}h$



G4Ellipsoid(name, a, b, c, z_{min}, z_{max})

Calculation of the Cubic volume uses the expression for the Ellipsoid cap volume:



$$V_{cap} = \frac{\pi ab}{3c^2} h^2(3c-h), h \le 2c$$

$$S_{cap} = \frac{\pi ab}{c^2} h(2c-h)$$ – area of the cap base

Lateral surface of G4Ellipsoid is described by the following expression:

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = 1$$

Lateral surface area is calculated by numerical evaluation of the following integral:

$$S = \int_0^{\frac{\pi}{2}} I(\varphi)d\varphi$$

Where $I(\varphi)$ depends on the following value:

$$k^2 = \frac{c^2}{a^2}\cos^2\varphi + \frac{c^2}{b^2}\sin^2\varphi$$

If $k^2 < 1$ then

$$I(\varphi) = \frac{2ab}{\sqrt{1-k^2}}\left[t\sqrt{k^2+t^2} + k^2 \sinh^{-1}\left(\frac{t}{k}\right)\right]_{t = \frac{z_{min}}{c}\sqrt{1-k^2}}^{t = \frac{z_{max}}{c}\sqrt{1-k^2}}$$

If $k^2 > 1$ then

$$I(\varphi) = \frac{2ab}{\sqrt{k^2-1}}\left[t\sqrt{k^2-t^2} + k^2 \sin^{-1}\left(\frac{t}{k}\right)\right]_{t = \frac{z_{min}}{c}\sqrt{k^2-1}}^{t = \frac{z_{max}}{c}\sqrt{k^2-1}}$$

If $k^2 = 1$ then

$$I(\varphi) = 4ab\,\frac{(z_{max} - z_{min})}{c}$$

If $a = b$ then k and I do not depend on φ, and the surface area can be calculated analytically:

$$S = \frac{\pi}{2} I$$

Summary. Key improvements in Geant4 11.01

- Analytical expressions have been obtained and used for the computation of the Surface area in G4Hype, G4TwistedTube, G4TwistedBox, G4TwistedTrd
- Fast numerical integration have been applied for the computation of the Surface area in G4TwistedTrap, G4GenericTrap, G4Ellipsoid
- Latest developments allow perform computation of the Cubic volume and Surface area in the rather optimal, fast and accurate way:
  - GetCubicVolume()
    - The MC method only in the Boolean solids
    - Numerical integration only in G4CutTubs
    - In all other solids – analytical expressions
  - GetSurfaceArea()
    - The MC method only in the Boolean solids and G4ScaledSolid
    - Numerical integration in G4CutTubs
    - Fast numerical integration in G4GenericTrap, G4TwistedTrap, G4Ellipsoid
    - In all other solids – analytical expressions
- Computation of the Cubic volume and Surface area is now in very good shape, and could be done even in the constructors. If so, then GetCubicVolume() and GetSurfaceArea() could become const.

Thank you!