

# HOLE

[Smart et al., 1993, Biophys. J., 65:2455-2460]

User specifies

- initial point  $p$  within channel
- vector  $v$  (approximately) in the direction of the channel

Uses Metropolis Monte Carlo simulated annealing to find the centre and radius of the largest sphere that can be placed within the channel with its centre on the plane perpendicular to  $v$  that passes through  $p$ .

Repeat for the next plane, at a fixed displacement from previous plane.

Stop when the accommodated sphere has a radius  $> 5 \text{ \AA}$ .

Repeat from  $p$  in the direction  $-v$ .

## Tilton et al., 1986, J. Mol. Biol., 192:443-456

Method to find channels within proteins

Atomic radii reduced by  $\Delta r$ , where:

$$(\Delta r)^2 = \frac{B}{8\pi^2}$$

Uses iterative procedure to find the largest sphere that can be inscribed by four atoms.

Intersections of these spheres define connections, the size of which is given by the circle of intersection.