Joint ICTP-IAEA Workshop on Monte Carlo Radiation Transport and Associated Data Needs for Medical Applications
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Lecture 21

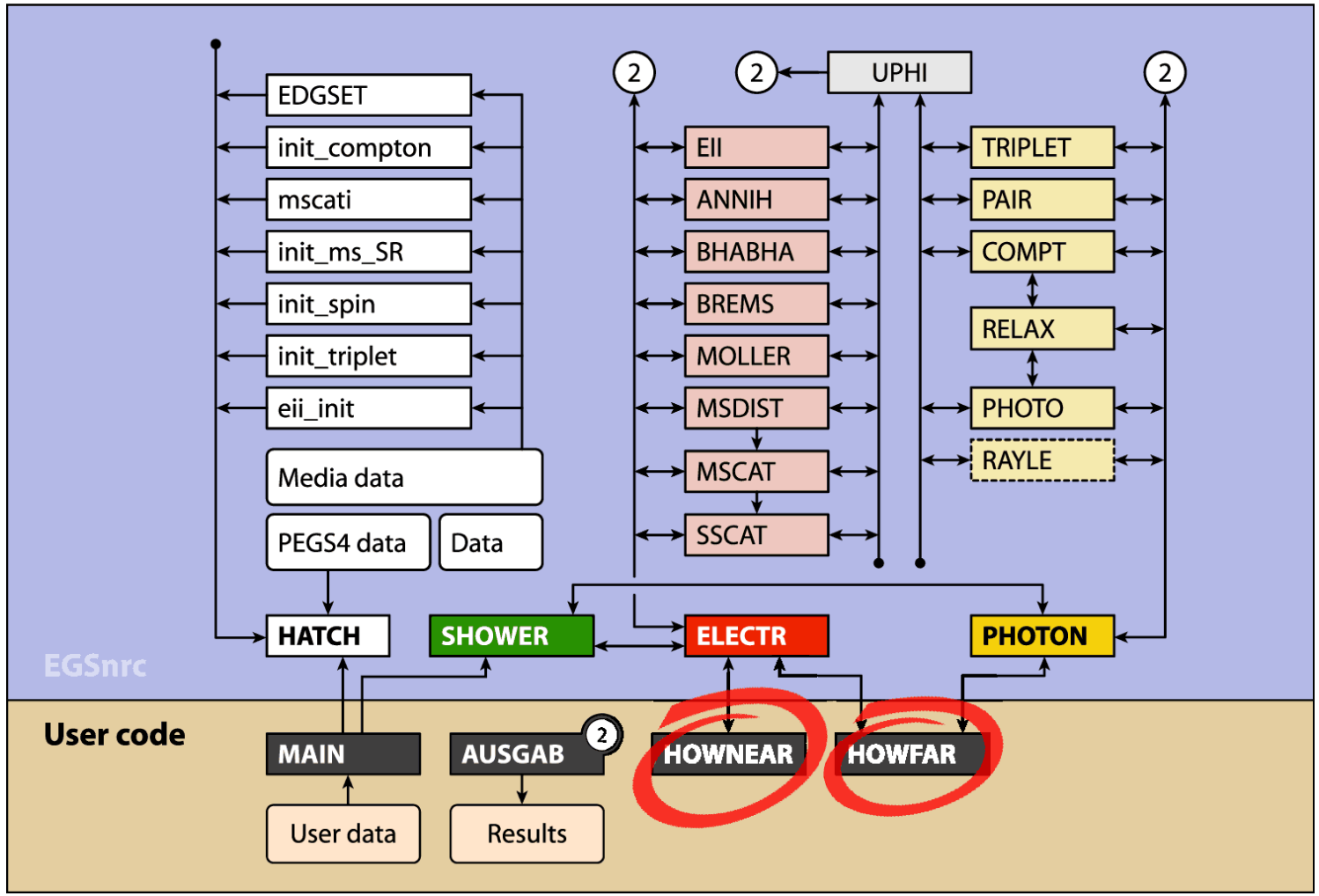
Fundamental geometry definition: howfar()and hownear()

Patricia Oliver

Nova Scotia Health
Dalhousie University

(This talk is based on slides from Frédéric Tessier)

`howfar()` and `hownear()` are part of the geometry

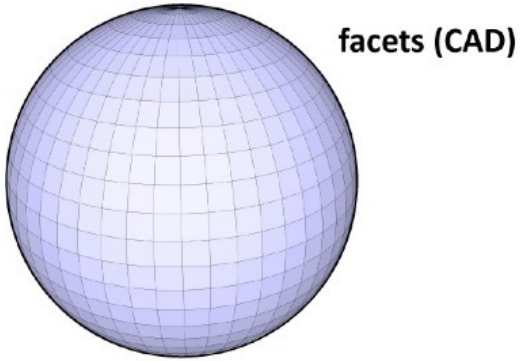


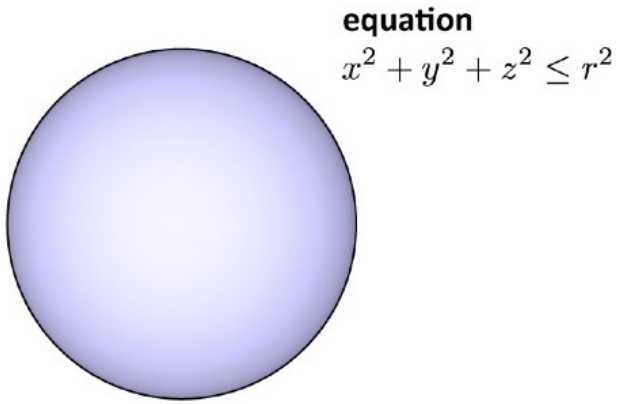
Decoupling of physics and geometry

- **EGSnrc** only concerns itself with transport of particles in infinite media.
  - EGSnrc only needs to know the composition of the medium that the particles are being transported in
- **User code** handles geometry

`howfar()` defines your geometry

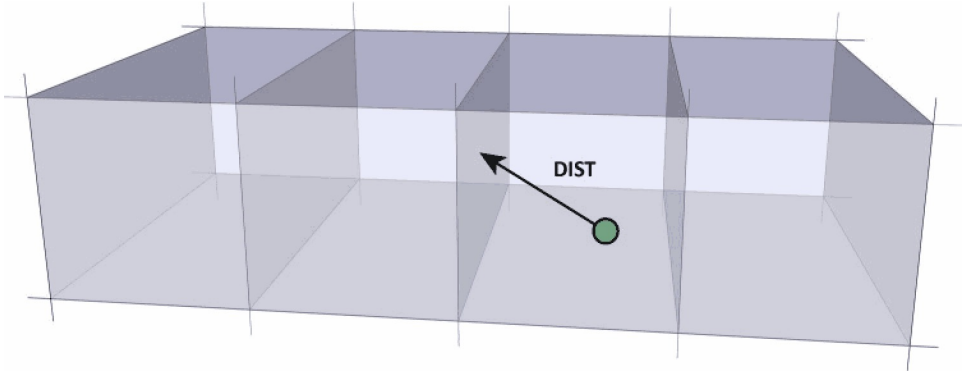
- Called by `ELECTR` and `PHOTON` EGSnrc subroutines before a particle step.
- Inputs to `howfar()`: region number, particle position, particle direction and `USTEP`
- `USTEP` is the straight-line distance over which EGSnrc **wants** to transport the particle (if there were no geometrical boundaries).
  - `USTEP` is based on the physics of radiation transport in infinite media (e.g., based on attenuation coefficients for photons) plus any other step-size constraints that the user may specify (e.g., `ESTEPE`, the max fractional energy loss per charged particle step)
- EGSnrc relies on a *functional representation* of geometry to determine whether a boundary will be crossed.





`howfar()` calculates distance

1. Call `howfar()` to determine `DIST`, the distance from the current particle position to the nearest geometric region boundary, along the particle's trajectory.



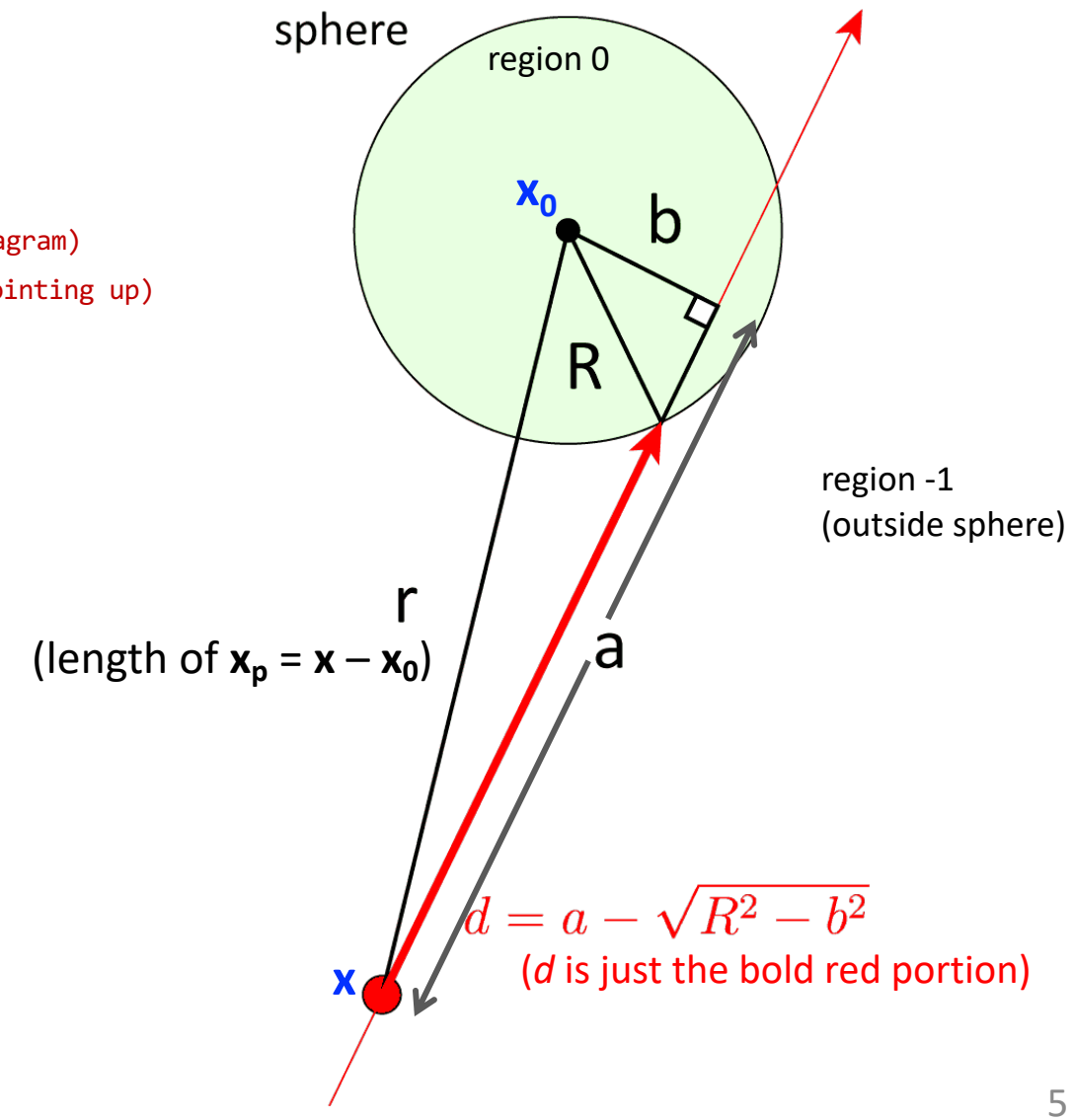
2. If `DIST` $\leq$ `USTEP` (the particle hits a boundary):
   - Set `USTEP = DIST`
   - Set `IRNEW = [the new region number]`

   } i.e., shorten the step so that the particle arrives exactly at the boundary

3. If the new region is outside the defined world (`IRNEW = -1`), mark it for discarding by setting the flag `IDISC = 1`.
4. Otherwise, transport the particle by `USTEP`.

Example: sphere `howfar()`

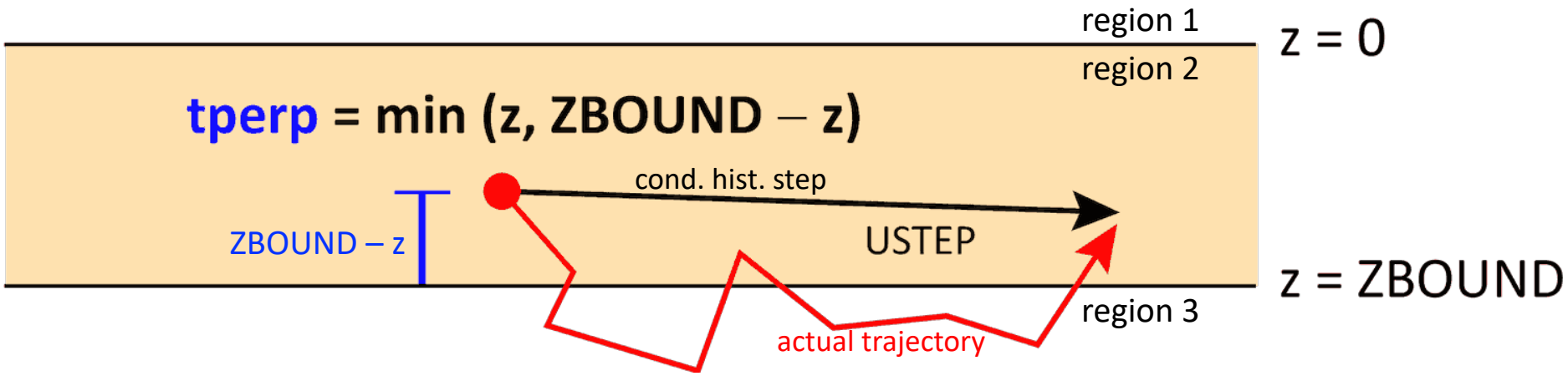
```
int EGS_cSpheres::howfar
        ( int ireg, const EGS_Vector &x,
          const EGS_Vector &u, EGS_Float &t,
          int *newmed, EGS_Vector *normal ) {

    EGS_Vector xp = x-x0; // xp points from x0 to x (pointing down in the diagram)
    double a  = xp*u; // u is a unit vector along the particle's trajectory (pointing up)
    double a2 = a*a;
    double r2 = xp.length2();
    double b2 = r2-a2;
    (...)
    else {   // not inside sphere (ireg<0)
        if (a < 0) {   // going towards sphere
            if (R2-b2 > 0) {   // intersect sphere!
                d = -a - sqrt(R2-b2);
            }
        }
    }
    if (d <= t) {  // DIST ≤ USTEP
        t = d;
        return nreg-1;  // region corresponding to inside sphere
    }
    return ireg;
}
```



`hownear()` is needed for electron transport

- The `hownear()` method computes the closest distance `tperp` to any surface in the geometry, from the current location of the particle, **in any direction**.
- When an electron takes a step close to a boundary, it is necessary to turn off multiple scattering to model the electron trajectory faithfully.

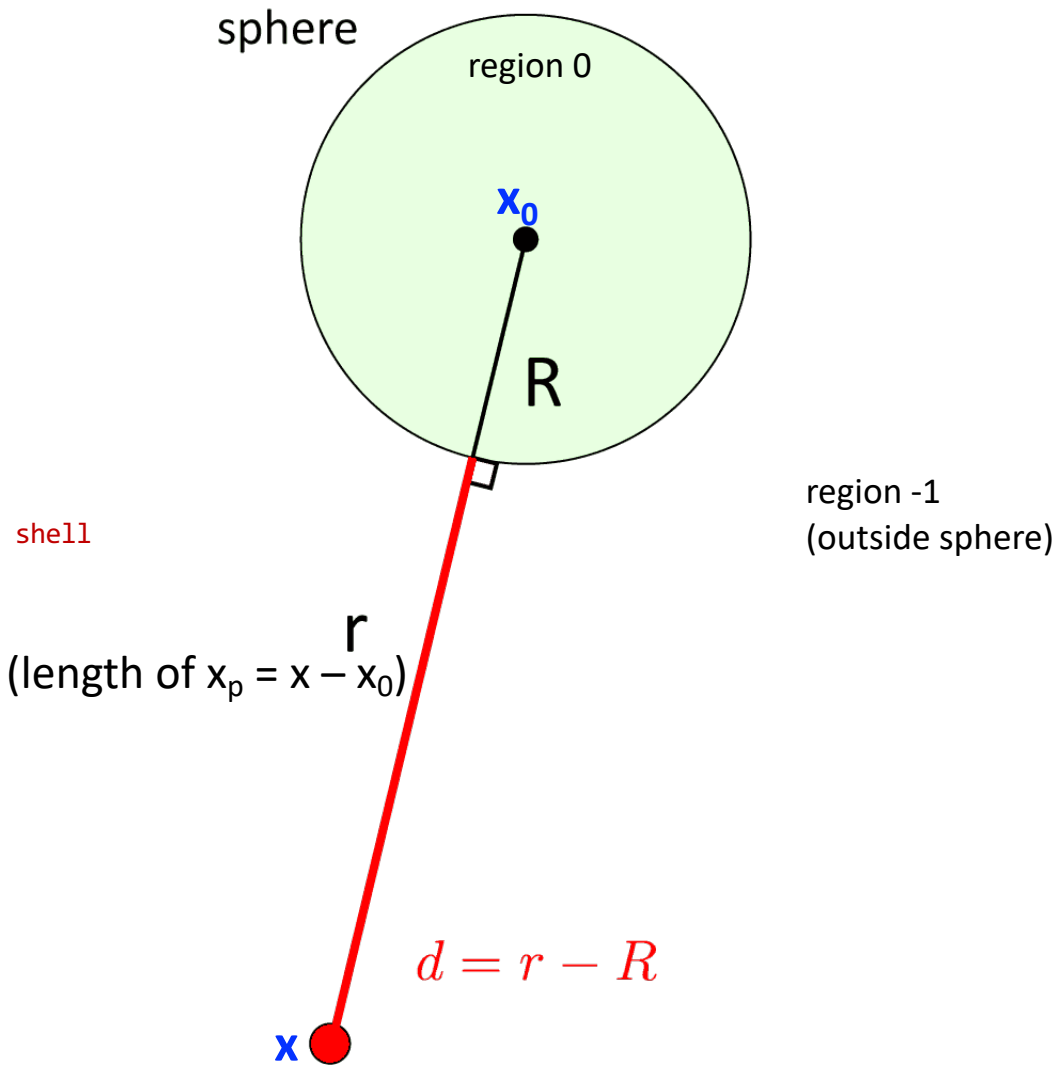
If not handled properly, condensed history steps near an interface can lead to incorrect dose in both regions, and incorrect particle transport (if the two media differ).




```
SUBROUTINE HOWNEAR (tperp, x, y, z, irl);   "from tutor1.mortran"
...
IF      (irl = 3) [ OUTPUT; ('Called HOWNEAR in region 3'); RETURN; ]
ELSEIF (irl = 2) [ tperp = min(z,(ZBOUND-z)); ]
ELSEIF (irl = 1) [ OUTPUT; ('Called HOWNEAR in region 1'); RETURN; ]
END;
```

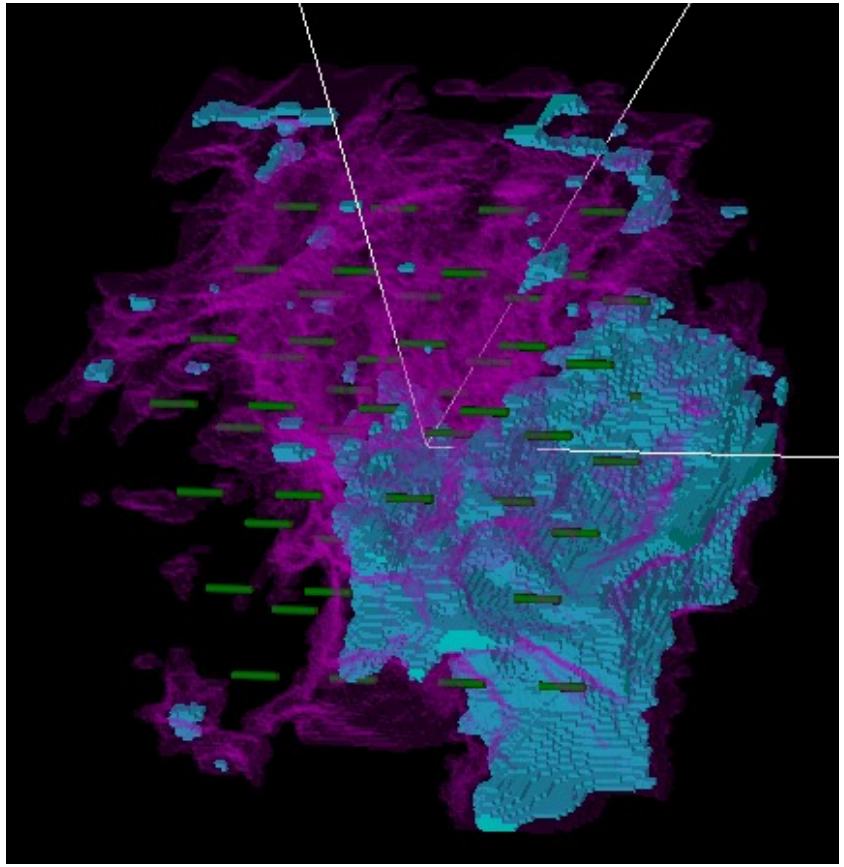
Example: sphere `hownear()`

```
EGS_Float EGS_cSpheres::hownear // a set of concentric spheres…
        ( int ireg, const EGS_Vector &x ) {

    EGS_Vector xp = x-xo;
    EGS_Float  r = xp.length();
    EGS_Float  d;

    // inside
    if (ireg >= 0) {
        d = R[ireg]-r;  // d > 0 because we are inside a sphere
        if (ireg) {  // if it's a set of concentric spheres
            EGS_Float dd = r-R[ireg-1]; // dd > 0 because we are in the shell
            if (dd < d) {
                d = dd;   // take the smallest distance
            }
        }
    }
    // outside
    else {
        d = r - R[nreg-1];
    }

    return d;
}
```



What about complex geometries?

- Elementary geometries can be combined to form composite geometries. Simulations will be **slower** if `howfar()` has to navigate through a complex hierarchy of geometries.

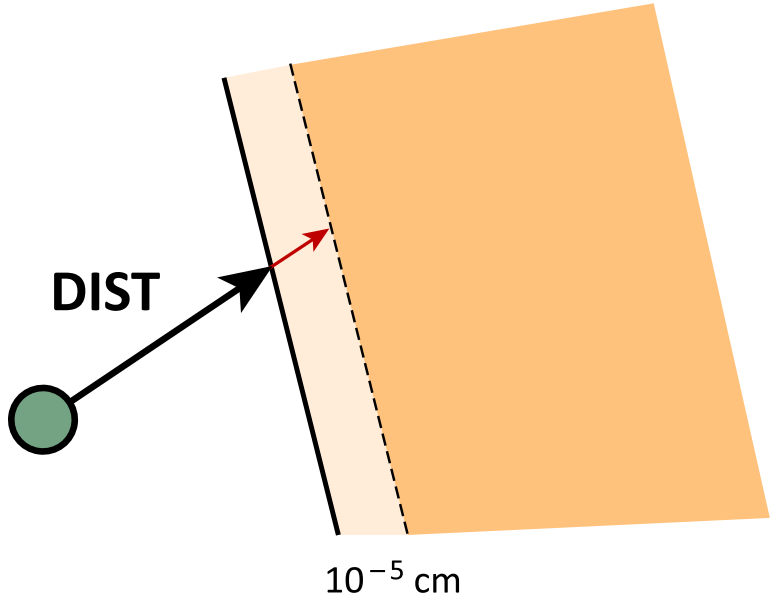


Example from egs_brachy manual: breast LDR simulation with voxelized tissue geometry and 64 seeds

Boundary crossing

- EGSnrc applications typically do **not** impose “fuzzy" boundaries to ensure that particles cross region boundaries (but BEAMnrc does!):
  - The particle is placed exactly at the boundary (i.e., `USTEP = DIST`)
  - This can lead to **rounding errors** due to the finite precision of floating point numbers
    → Position of particle is in conflict with region number

- **Errors** in `howfar()` typically show up as negative `USTEP` errors.

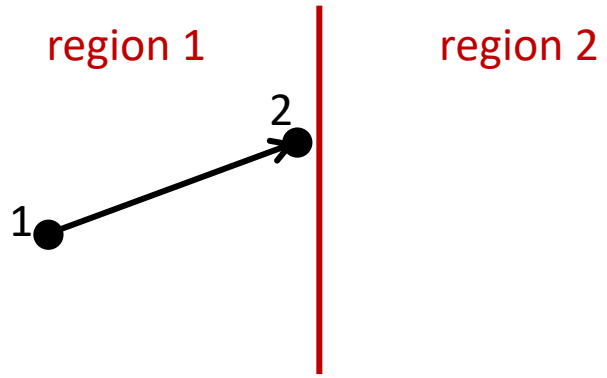


Fuzzy boundaries in BEAMnrc: particle is “pushed” an additional small distance to avoid rounding errors

Floating point rounding errors

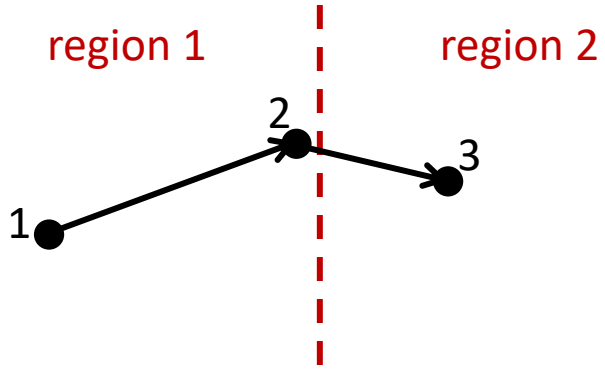
Example:

- Particle is in region 1 and is directed toward region 2
- `howfar()` is called with `USTEP` large enough to escape region 1
  - `USTEP = DIST` and the particle is at the interface between regions 1 and 2
  - The current region is updated: `IRNEW = 2`
- Consider the case where rounding errors result in an **undershoot**
  - The particle's region number is 2 but its position corresponds to region 1!



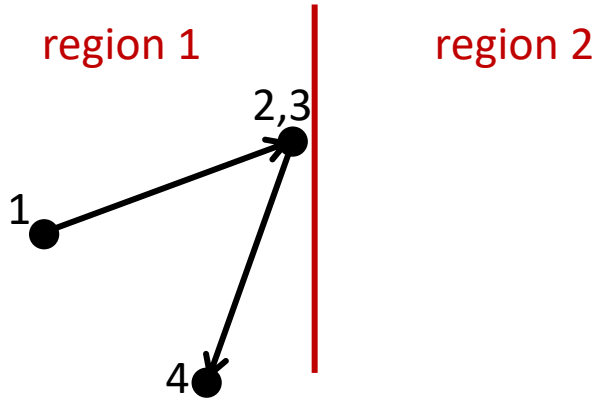
Floating point rounding errors

- In general, if there is a contradiction between the particle's region number and (x, y, z) position:
  - **Case #1**: If the particle is still headed in the direction of the surface, then this surface is ignored, as if the particle had already crossed.

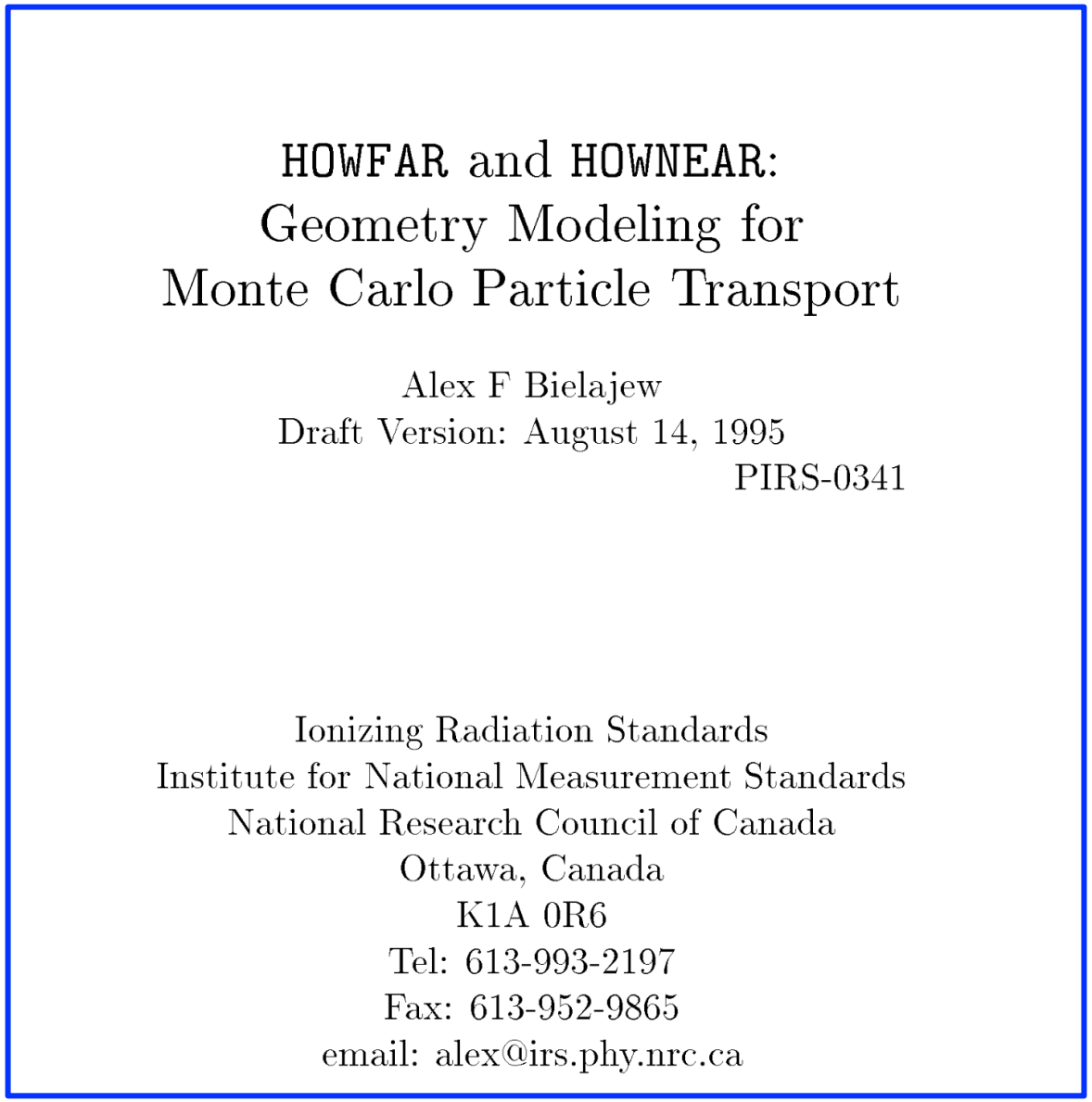


Floating point rounding errors

- In general, if there is a contradiction between the particle's region number and (x, y, z) position:
  - **Case #2**: If the particle is headed away from the surface, then `howfar()` will return a small **negative** number for `USTEP`
    - To resolve this, `USTEP` is set to zero, and the surface is assumed to be crossed again:
      `IRNEW = 2` → `1`
    - On the next step, the particle may continue its backscatter trajectory in region 1
      - Position and region number are no longer in conflict



Where to learn more



HOWFAR and HOWNEAR:
Geometry Modeling for
Monte Carlo Particle Transport

Alex F Bielajew
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Ionizing Radiation Standards
Institute for National Measurement Standards
National Research Council of Canada
Ottawa, Canada
K1A 0R6
Tel: 613-993-2197
Fax: 613-952-9865
email: alex@irs.phy.nrc.ca