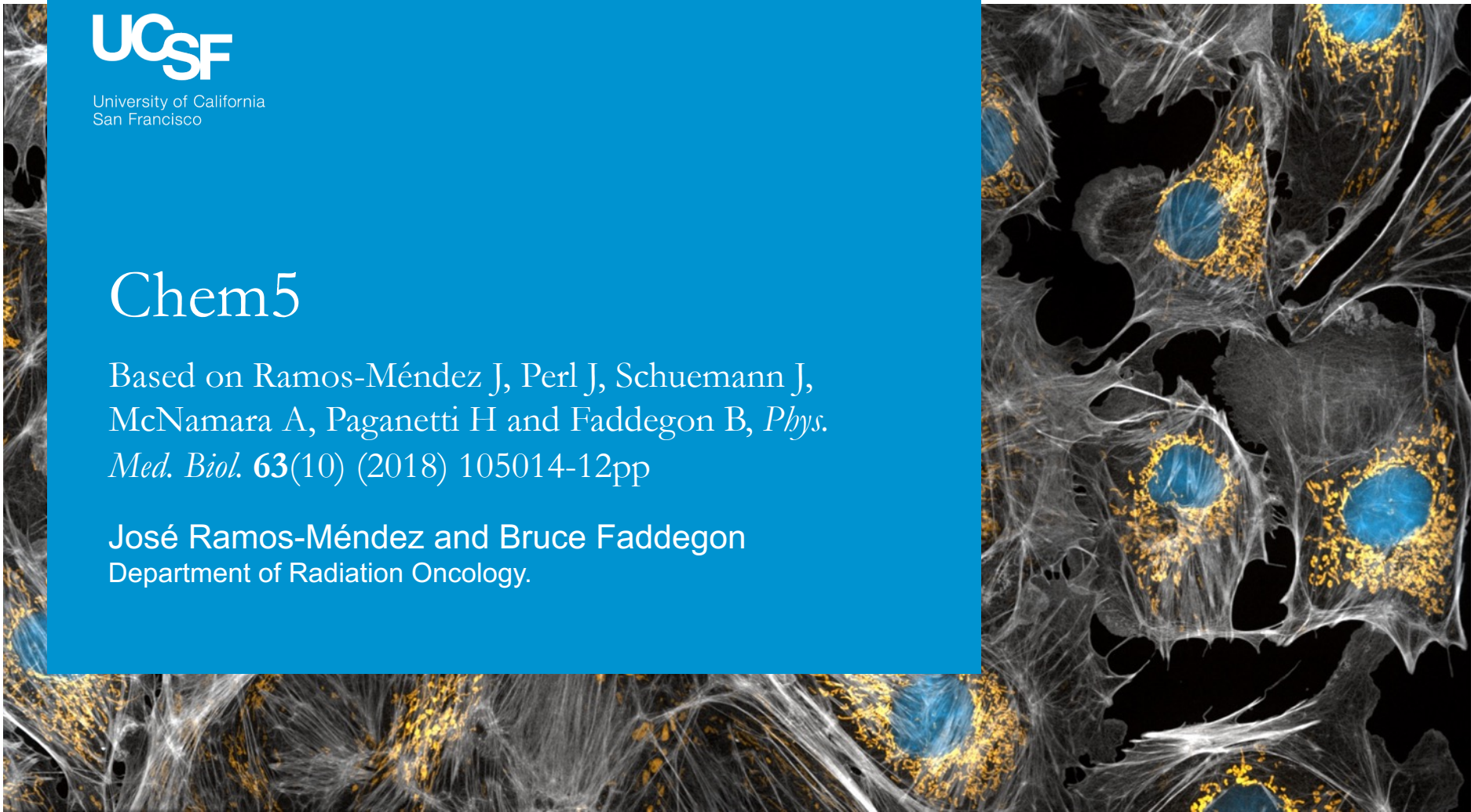


University of California
San Francisco

Chem5

Based on Ramos-Méndez J, Perl J, Schuemann J, McNamara A, Paganetti H and Faddegon B, *Phys. Med. Biol.* **63**(10) (2018) 105014-12pp

José Ramos-Méndez and Bruce Faddegon
Department of Radiation Oncology.

Geometry

- The example is a modified version of chem4.
- The world volume is a simple box which represents a “pseudo infinite” homogeneous medium.
- Two parameters define the geometry:
  - the material of the box -- for Geant4-DNA it must to be water.
  - the full size of the box.

Physics and chemistry lists.

- Geant4 modular list introducing two constructors:
  - G4EmDNAPhysics_option8
    - Born for inelastic scattering.
    - CPA100 for elastic scattering.
  - G4EmDNAChemistry_option1.
    - Diffusion coefficients and reaction rates used by RE/RITRACKS
    - The thermalization distance of e^-_{aq} can be selected using G4EmParameters (Thanks Mathieu!).
    - The example uses Ritchie's model (Ramos-Méndez, et al., 2018 PMB)

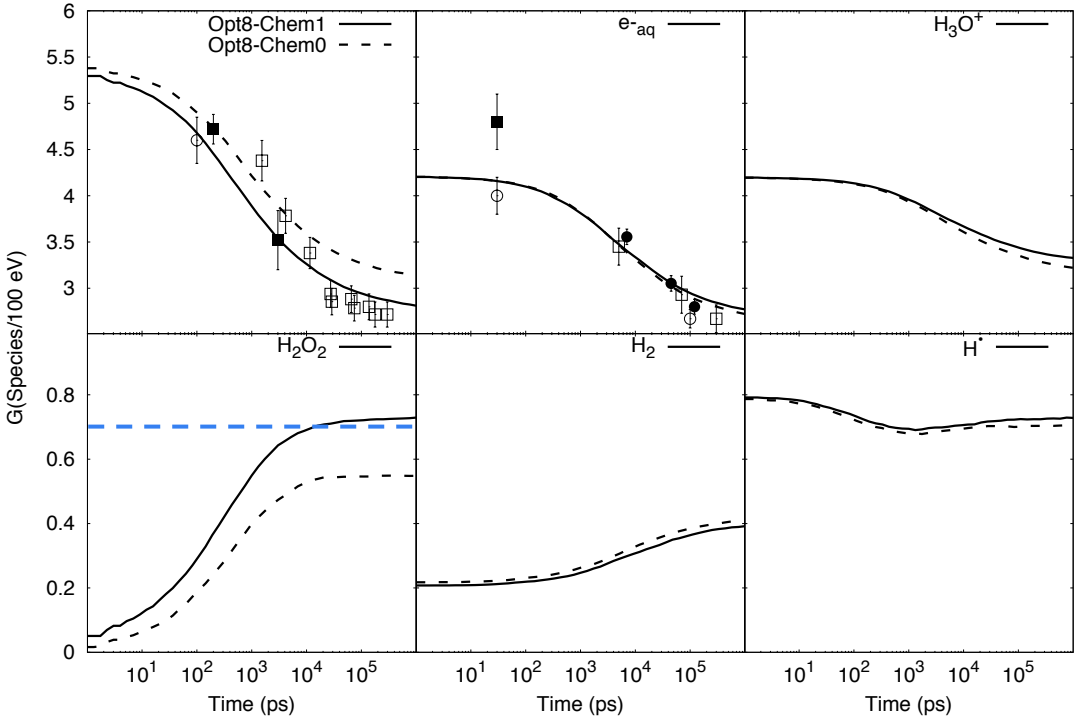
Scoring

- G-values (number of chemical species created per 100 eV) are retrieved using e– of 1 MeV.
- The primary e– is terminated after 10 keV of its energy is deposited. Secondary e– are transported down to the physics model limits.

```
# after 10 keV of energy loss by the primary particle, the primary is killed
                /primaryKiller/eLossMin 10 keV
 # if the primary particle losses more than 10.1 keV, the event is aborted
                /primaryKiller/eLossMax 10.1 keV
```

Output

- Tabulated data in ASCII format:
  - Time [ps] G-value (/eV) RMS Molecule's name.
- A GNUplot script is provided to display G-values vs log-scale time (in ps).
- Reference experimental data for $^{\bullet}OH$ and e^{-}_{aq} available in
  - chem5/data/



For a comprehensive study on chemistry and physical parameters, see Wook-Geun's presentation in Parallel 8A

UCSF

UCSF