

American Crystallographic Association (ACA) Annual Meeting, Cincinnati, OH, July 20-24, 2019

# Michael Rossmann (1930-2019): phase extension and *ab initio* phasing

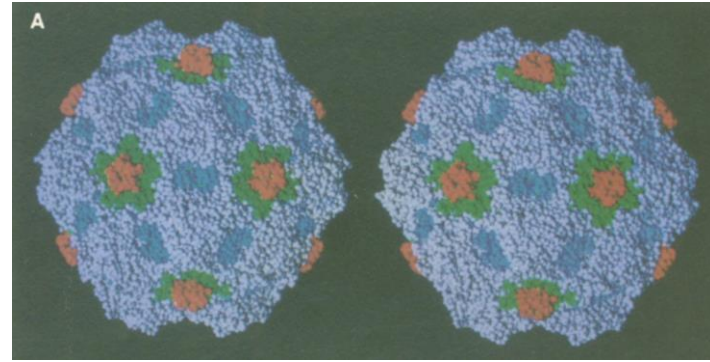
1988 -  
1992



Hao Wu, Ph.D.  
Harvard Medical School  
Boston Children's Hospital

# Canine Parvovirus (CPV)

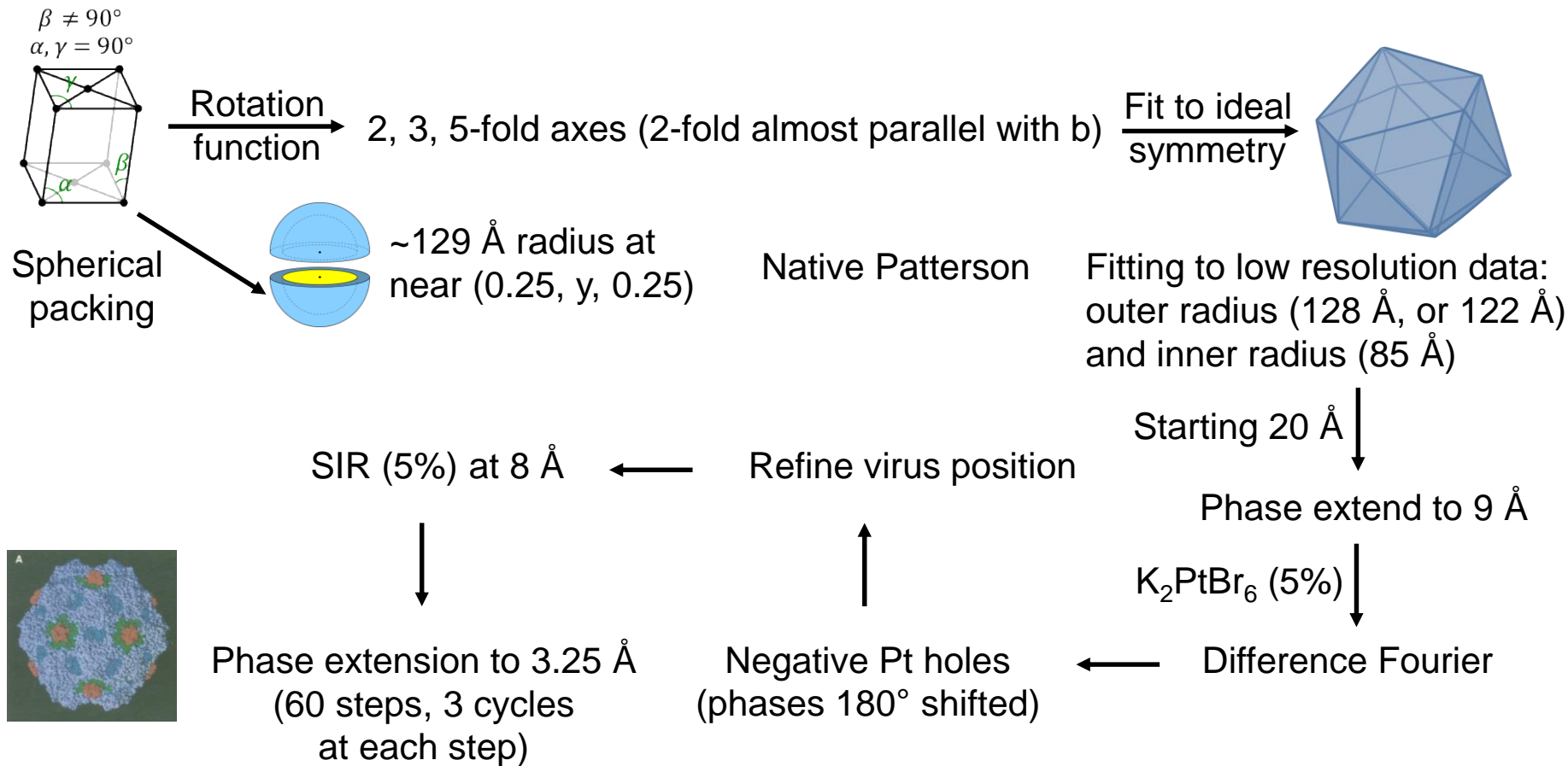
- Full particle and empty capsids: Jun Tsao, Hao Wu, Michael Chapman, Mavis Agbandje, Walter Keller, Kathy Smith, Ming Luo, Tom Smith, Richard Compans, Colin Parrish.
- Parvoviruses negative sense ssDNA viruses and are pathogenic.
- Canine parvovirus is a remarkable example of the emergence of a new viral pathogen, likely from feline panleukopenia virus (FPV).
  - Identified in 1978; become pandemic in a few months; endemic in all populations of domestic and wild canids that have been examined.
  - Genetic recombination mapping shows that four coding and three noncoding changes within the coat protein region can endow FPV with the ability to replicate in dogs.



# Structure determination of CPV: data collection

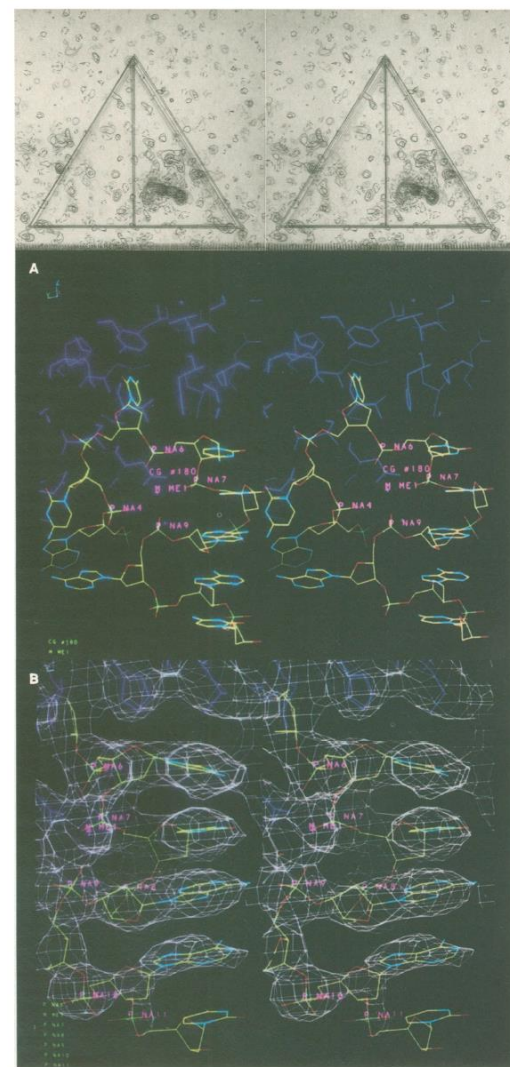
- Icosahedral symmetry with triangulation number (T) = 1.
- $P2_1$  with cell dimensions  $a = 263.1$ ,  $b = 348.9$ ,  $c = 267.2$  Å, and  $\beta = 90.8^\circ$
- Data collected at CHESS and Daresbury.
  - Oscillation angles from  $0.3^\circ$  to  $0.7^\circ$ ;  $> 2.8$  Å resolution; one virion/au.
  - Very low resolution data collected by increasing the crystal-to-film distance from 100 to 300 mm
- Crystals were randomly oriented, indexed by the auto-indexing procedure of Sangsoo Kim developed while at Purdue.
- Refinement of crystal orientation, intensity measurements, scaling, post-refinement, and averaging were accomplished with the Purdue processing program package.
- Latter two formed some of the basis for modern data processing software.

# Structure determination of CPV: *ab initio* phasing



# Structure determination of CPV: model building and DNA

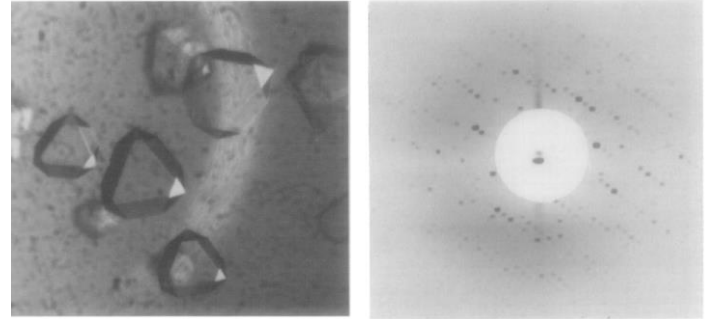
- Traced and sequence fitted on a stack of transparencies; Wrong hand; FRODO (T. A. Jones).
- Most of the nucleic acid (as in other spherical viruses) is not seen. In CPV some DNA structure is visible where icosahedral symmetry has been imposed on it by internal binding to the coat protein.
- A total of 11 nucleotides were built into this density. Since this occurs in each of the 60 icosahedral asymmetric units of the virus, there are a total of 660 visible bases, or 13 percent of all of the encapsidated DNA.



# Influence of a life time

- Michael was a virtuoso in solving structures
  - Advanced crystallography course, Thursday evening discussion, working closely with us – synchrotron trips, project discussions, Fortran programming, writing papers
- Support us to go to meetings
- Support us for collaborations:
  - 1) John Innes Institute, UK
  - 2) University of Kentucky
- Personal development
  - Always interested in you; in order to graduate: swimming, driving
- Unwavering enthusiasm for life and almost childlike curiosity

Cauliflower mosaic virus (CaMV)



# Tributes to Michael Rossmann: Let the legacy continue

- Arnold E, Wu H, Johnson JE (2019). Michael G. Rossmann (1930-2019), pioneer in macromolecular and virus crystallography: scientist, mentor and friend. ***Acta Crystallogr D Struct Biol.*** 75: 523-527
- Wu H, Arnold E (2019). Michael G. Rossmann (1930-2019). ***Nat Struct Mol Biol.*** [Epub ahead of print]
- Chuan (River) Xiao, Liang Tong (2019). Michael G. Rossmann (1930-2019). ***Structure*** in press
- Johnson JE (2019)...
- ....



# Mila Mountain (Lhasa, Tibet) 2012





Zhangjiajie, 2011



Japan, 2008



Morocco, 2009



Lhasa, 2012





# Parade of Students: Rossmann Symposium 2017

