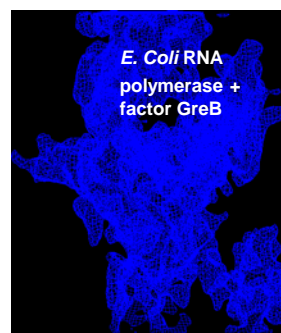
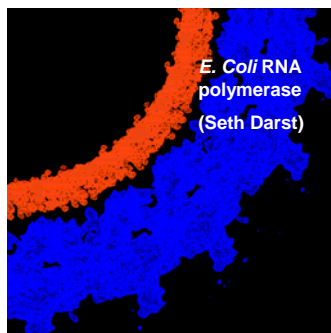


Note: Situs classic, correlation, and multi fragment docking tutorials are documented online at <http://situs.biomachina.org/ftut.html>

Shown in the following are Dr. Wriggers' extra slides for

Useful Map Tools in *Situs*

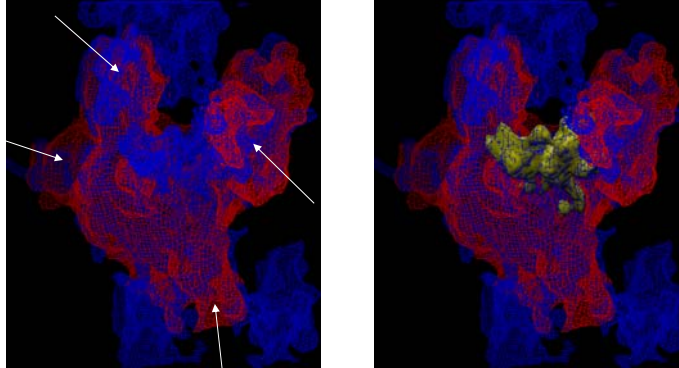
Registration of Two EM Maps



Problem: different helical arrays

Need to perform difference mapping to localize GreB (difficult at variable helical symmetry)

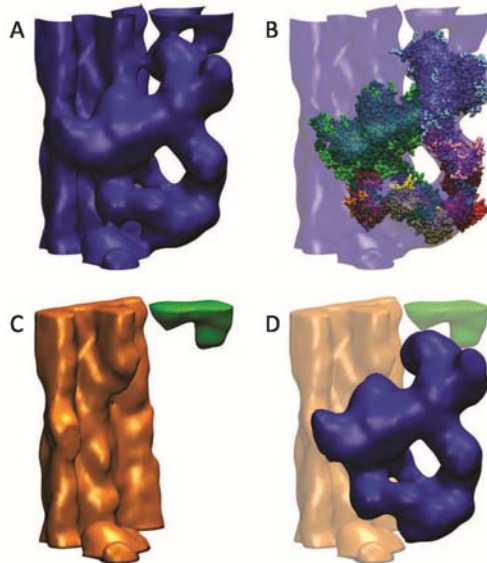
Registration and Difference Mapping



Rigid-body docking: The RNAP “jaws” are open in presence of GrepB factor, perform flexible map fitting

Work flow: vol2pdb (conversion to pdb), colores (rigid-body fit), qplasty (flexible fit), voldiff (difference map)

VolEdit, VolDiff: “Map Algebra”

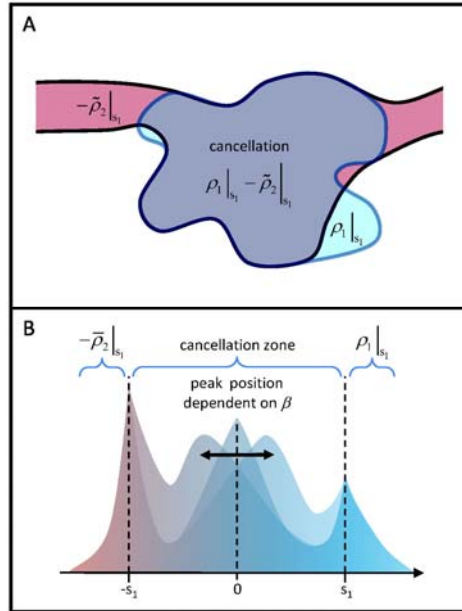


Wriggers, Alamo
& Padrón,
J. Struct. Biol.,
173:445, 2011

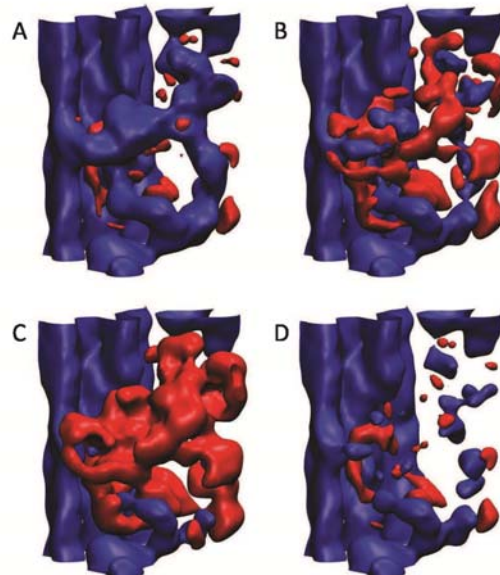
VolHist: Histogram Matching

$$\begin{aligned}\tilde{\rho}_2(\beta) &= \sigma(\beta) \cdot \rho_2 + \beta, \\ \sigma(\beta) &= \frac{s_1 - \beta}{s_2}, \\ \Delta_{12}(\beta) &= \rho_1|_{s_1} - \tilde{\rho}_2|_{s_1}(\beta).\end{aligned}$$

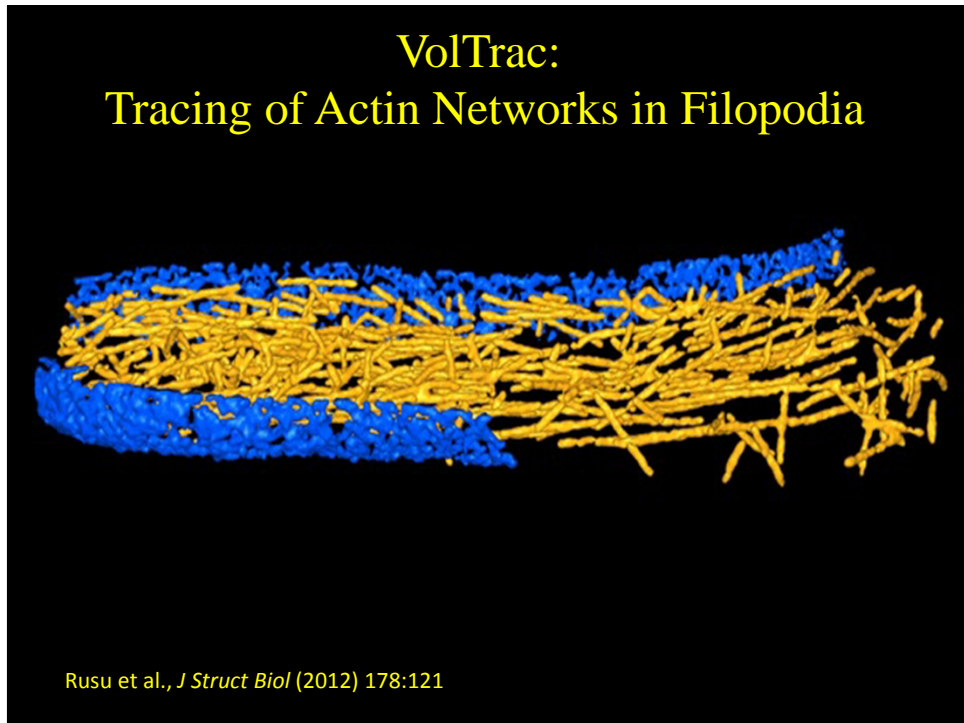
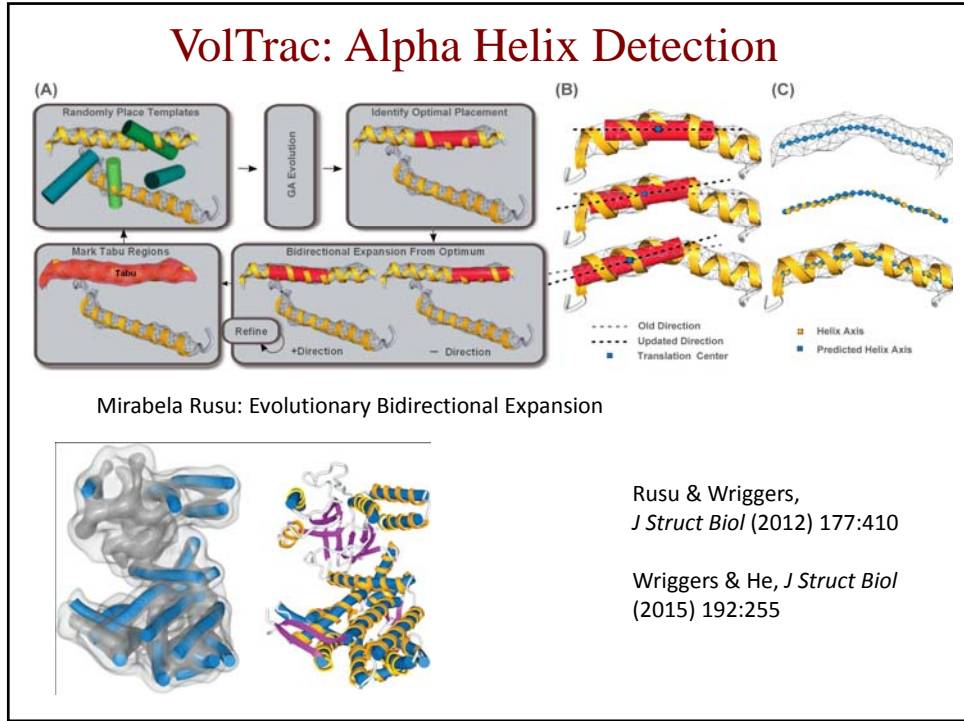
Wriggers, Alamo & Padrón, *J. Struct. Biol.*, 173:445, 2011



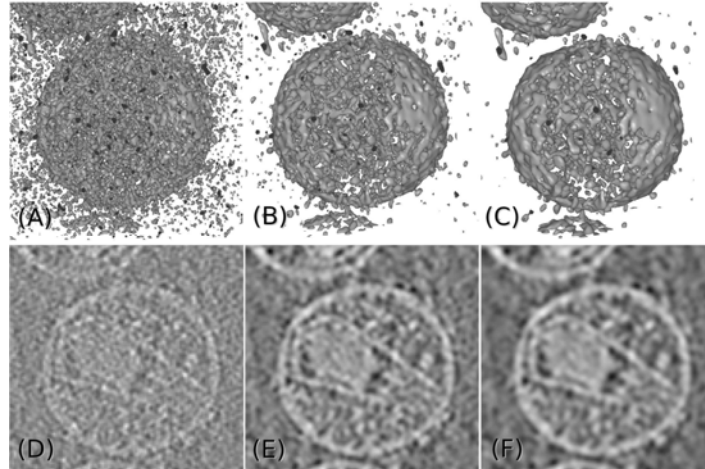
Histogram Matching with Gain and Bias



Wriggers, Alamo & Padrón, *J. Struct. Biol.*, 173:445, 2011



VolFiltr: Denoising of Maps and Image Stacks



Variance-Based Supervised Digital Path Classification (Situs 2.7 / Sculptor 2.1) Starosolski et al., *Biophysical Reviews* 2012; 4:223