SIMPLE 2017 Development Document

Responsibilities: Hans, Cyril, Michael?, Susan&Hans

RANDOM STUFF

* Multi-state with different point-groups (all subgroups)
* Need to have another go at unsupervised picking (massively parallel mass-centring)
* Class for memory allocation simple\_alloc. Keep track of mem exceptions and profile memory (hash table).
* Go over all random number generations and see if we can use matrices instead
* Replace integer random number generator with intrinsic one (Guide to Fortran 2008)
* mailx -s "mail from prime2D" hans.elmlund@monash.edu < from\_prime2D

NEW DEVELOPMENTS

* Probabilistic SO(3) scatter search for high-resolution refinement
* implement tilt test
* Fractional particle update with learning rate. Say we have 50,000 images and select to update 5000 every round. The probability for updates should be initialised to 1/nptcls and then updated 1/#updates per particle and normalised. Instead of subtracting and updating, we simply keep the current set of Fourier coefficients on disk (normalised and gridding corrected) and update the model with a learning rate 5,000/50,000=0.1, for the new and 45,000/50,000 =0.9 for the old. Probably the fraction should be given as a fraction of total # particles, 10-20%. This should take state=0 particles into account.

EXCEPTION HANDLING

* exception handling class that makes more sensible outputs (especially when running the code in distributed mode). We need to create a database of exceptions and then have ONE control point where we check the stack for errors and report what has failed (similar to the command line dictionary). JOB)\_FINISHED should communicate

Known bugs

None at the moment

Compilation

* port to ifort (Intel compiler)
* port to PGI (Portland group, with CUDA-FORTAN)

Documentation

Need to get a html code doc generator in place and fix the doc of every class. Will FORD source code documentation provide the solution?

<http://fortranwiki.org/fortran/show/FORD>

<https://github.com/cmacmackin/ford>

<http://jacobwilliams.github.io/json-fortran/index.html>

Books/webpages

* Structured parallel programming
* Structure and Interpretation of Computer Programs
* J-P Morrison. Flow-Based Programming: A New Approach to Application Developments. CreateSpace, 2nd ed.
* Mathematical Foundations of Imaging, Tomography and Wavefield Inversion
* Geometric Algebra for Computer Science (Revised Edition): An Object-Oriented Approach to Geometry (The Morgan Kaufmann Series in Computer Graphics) 1st Edition
* The Princeton Companion to Applied Mathematics
* Practical Machine Learning: http://www.computervisionmodels.com/
* Applied Stochastic Modelling, Second Edition (Chapman & Hall/CRC Texts in Statistical Science) 2nd Edition http://szeliski.org/Book/