SIMPLE 2017 Development Document

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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

* implement tilt test

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>