2013
international year of crystallography

Technical editing and house style

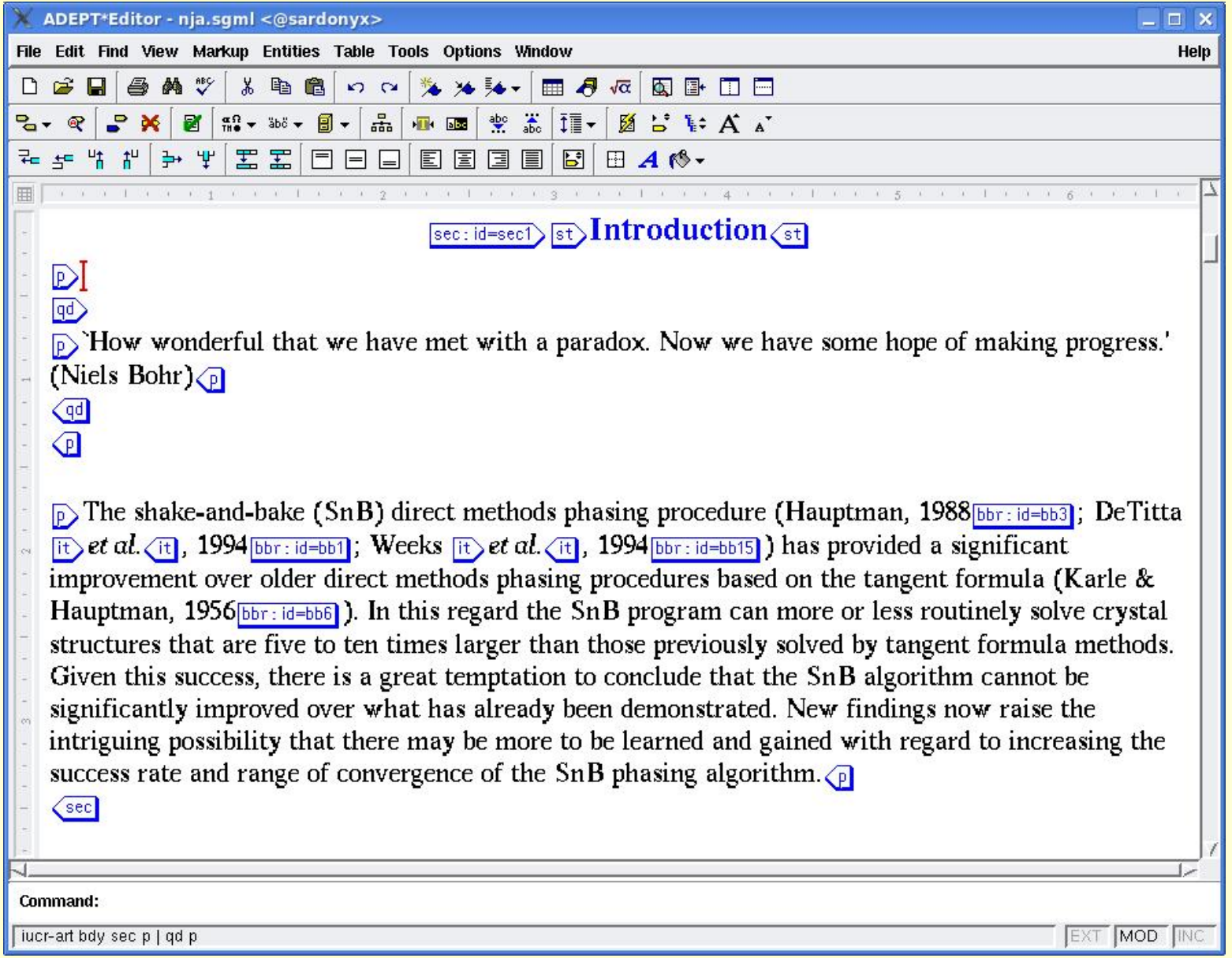
Nicola Ashcroft

Crystallography Journals Online

Starting point for technical editing

- Text, tables and figure captions in one SGML file
- Equations within the SGML as plain TeX fragments
- SGML conforms to our DTD
- Figures as tiffs, one file per figure

Crystallography Journals Online



Crystallography Journals Online

First edit in Adept

Abstract suitable for abstracting services

British/American spellings?

Grammar, punctuation – query if unclear

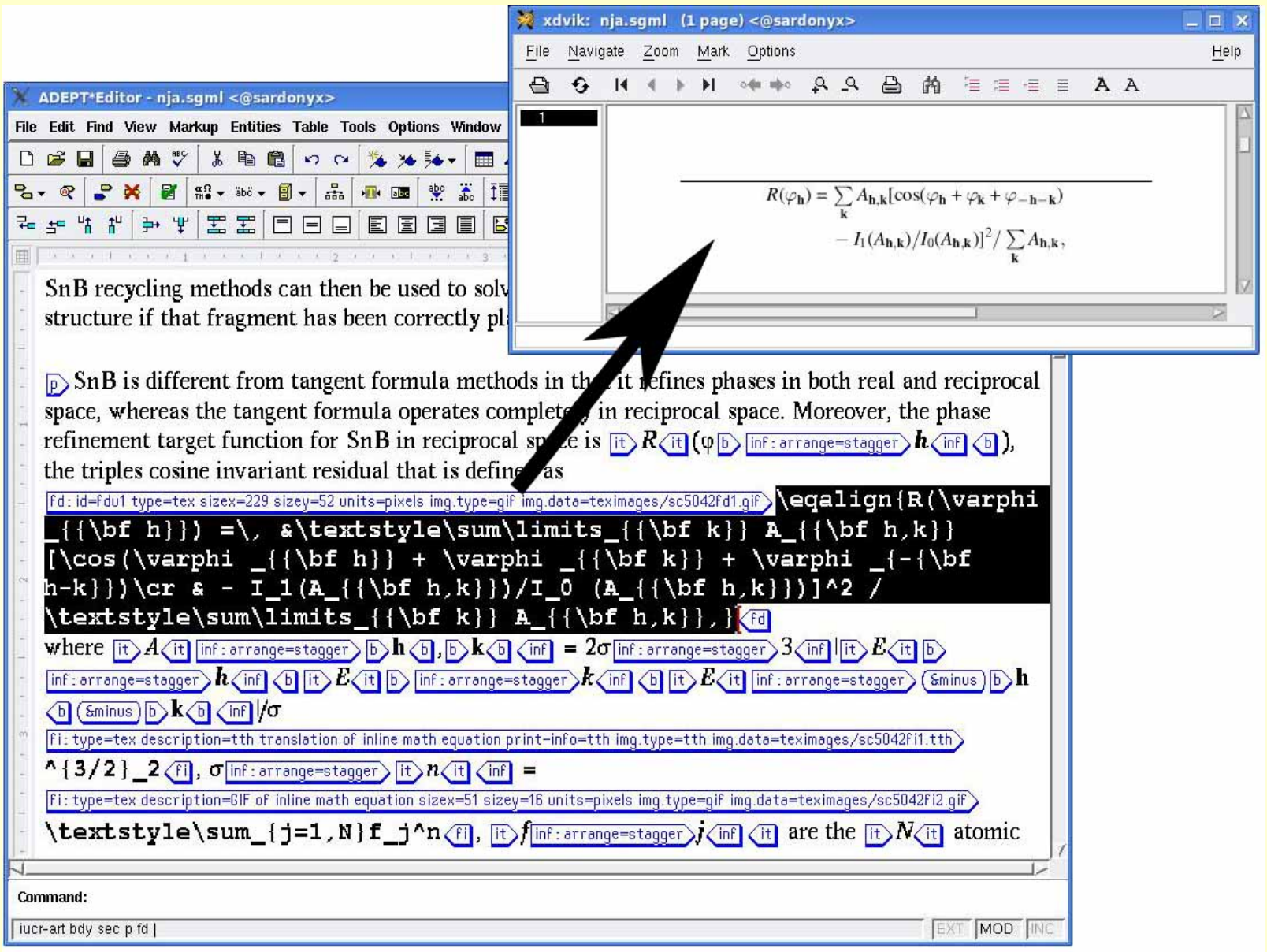
Abbreviations defined?

House style

Check URLs

Equations (in TeX) can be previewed

Crystallography Journals Online



Crystallography Journals Online

Page make-up software (3B2)

- Reads in and displays SGML for text
- Reads in tiffs for figures
- Interprets and displays TeX
- Figures and tables placed at top or bottom of pages, text flows around them
- Outputs PostScript for pdfs for proofs

Crystallography Journals Online

3B2 Total Publishing System

File Edit View Document Page Frame Styles Text Graphic Window Help

SGML | SGML menu | LMs | Table LMs | FormatA | Format | Find elem | SGML parse | SGML print | SGML in | SGML save | Gen | P | T | Help | SGML exit

/a/sc5042/sc5042.3d – changed

/abs
/app
/atl
/aug
/bdy
/bm
/ded
/doc-catgry
/edtrl-office
/enun
/fig
/H2
/index
/inf
/iucr-art
/misc
/organisers
/proc-tl
/qd
/role
/schmtex
/sec
/snm
/st
/tfn
/tgroup
/unl
_actacontru
deflt
_runheadsty
_runninghea
_suserscript
abs
abs-agenci
absparstyle
acc
accactae
accline
accold
ack
ackstyle
actacontrur
actajournal
addresssty
addtoissued
alpha
app
apphead1st
appm
atl
au
au-notes
aug
aunmarker
aunotestyle

3: rhead,–,– : rhead

research papers

8: linenumberstreamleft,–,– | 9: linenumberstreamleft,–,–

Table 1
Unrefined one-atom phase sets.

Phase errors, $\Delta\varphi = \langle|\varphi_{true} - \varphi_{trial}|\rangle$, were computed from the N one-atom sites for four light-atom structures containing no atom larger than oxygen. The number of phases used in the SnB analysis and the percentage of N trials that proceeded to solutions are given. The range, mean and standard deviations of the N sets are listed. Also listed is the percentage of phase sets, each undergoing 100 SnB cycles of random N-atom refinement, *excluding solutions*, that attain $\Delta\varphi$ less than 30 and 75°.

Structure	No. of atoms N	No. of φ's	No. of triples	% Solutions	$\Delta\varphi$ range (°)	$\Delta\varphi \pm$ standard deviation (°)	< 30° (%)	< 75° (%)	Reference
LLED	34	340	3000	34	63 → 37	73 ± 4	30	9	(a)
SILS4	95	300	9000	15	66 → 33	79 ± 5	28	5	(b)
TERN	116	700	7000	3	70 → 37	79 ± 4	31	3	(c)
SILS5	117	900	10000	9	68 → 39	82 ± 5	29	4	(d)

References: (a) Pletnev *et al.* (1980); (b) Pletnev *et al.* (1991); (c) Miller *et al.* (1993); (d) Pletnev *et al.* (1992).

methods expectation value of $\cos(\varphi_h + \varphi_k + \varphi_{-h-k})$ derived by Hauptman (1966) based on its A value. For an N-atom structure determination, one usually selects ca $10N$ E values and $100N$ triple phase invariants as the basis of phase refinement by the $R(\varphi_h)$ function.

An SnB phasing trial begins with randomly generating coordinates for an N-atom structure and using those positions to compute the initial phase values. Those phases are next refined by minimizing $R(\varphi_h)$, for each phase φ_h, while all others, φ_k and φ_{-h-k}, are temporarily held fixed until it is their turn to be refined. One of the simplest refinement schemes simply increments the value of φ_h by 0, ±90 and 180°, and accepts the value that produces the lowest value of $R(\varphi_h)$. Once all the phases have been adequately refined in this manner, an E map is computed and the N largest peaks are then chosen as the starting point for the next cycle of refinement. A sufficient number of cycles of refinement are performed to ensure convergence, at which time R_{min}, the overall value of $R(\varphi)$ for all the phases, will approach its global minimum. The value of R_{min} is generally significantly less than 0.5 for the correct solution, and greater than 0.5 for all the various non-solutions. A solution is usually not obtained in those instances where there is no clear separation in R_{min} values. Fig. 1 compares the progress of a typical SnB solution *versus* a non-solution with regard to the computed value of R_{min} and its associated average mean phase error, $\langle|\Delta\varphi|\rangle = \langle|\varphi_{true} - \varphi_{cal}|\rangle$, as a function of the SnB phase refinement cycle number.

Once a solution has been obtained, one characteristic of well determined phases is that the values of $R(\varphi_h)$ for the individual phases should increase dramatically upon perturbing the value of φ_h by 0, ±90, 180° from their solution values. Conversely, if there should be little difference among the four R values, then there would be no particular reason to believe that any one of the four permuted values would be any better than the other three. Having made this conjecture, one might also ask the same question with regard to SnB phase sets that have not fully converged to a recognizable solution. That is, might a large variance indicator for any $R(\varphi_h)$ still be correlated with how well that phase has converged toward its true value? We decided to examine this possibility.

5: dummy1,–,rg1 : floatframefig1

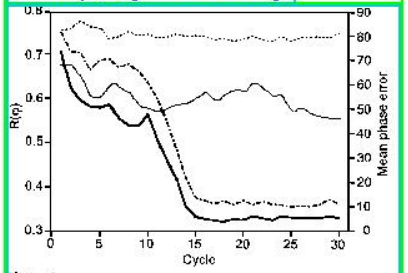


Figure 1
Example of the SnB progress of a solution *versus* a non-solution. The heavy line marks the value of R_{min} as a function of SnB cycle number for a solution, the value for R_{min} drops significantly below 0.5 at about cycle 10. The $\langle|\Delta\varphi|\rangle$ associated with this trial (dot-dashed line) rapidly decreases to ~10° once this is achieved. R_{min} for a typical non-solution (fine line) seldom reaches as low as 0.5, while its associated $\langle|\Delta\varphi|\rangle$ (dotted line) hovers near that for randomly generated phases in the vicinity of 85 to

3. Numerical tests

Four moderately large $P2_12_12_1$ structures each having about 100 non-H atoms in the primitive unit cell were selected. Firstly, it will be necessary to be able to evaluate $\langle|\Delta\varphi|\rangle$ for any SnB trial with the known structure relative to some unknown choice of origin and enantiomorph. It is a fairly trivial matter to do this in the space group $P2_12_12_1$ by simply examining the 16 permissible choices of origin and enantiomorph and selecting the choice with the smallest phase error. Secondly, it is well known as a point of interest that single-atom search models often generate initial trial sets with a significantly lower $\langle|\Delta\varphi|\rangle$ than N-atom models (Weeks *et al.*, 1994). Table 1 lists the one-atom phase errors for the starting sets of phases corresponding to each of the N atoms of the four known structures chosen. For the purpose of the following study we temporarily ignored all those single-atom starting sets that subsequently produced SnB solutions upon further refinement, or between 3 and 34% of all sets depending on the

7: filename,–,– : footer

Acta Cryst. (2011). A67, 430–434 | Langs and Hauptman • Direct methods | 431

SC5042 PROOFS

Pasteboard: pboard2

Tx sc5042 – 0(41184)c

<!DOCTYPE IUCR-ART PUBLIC "-//IUCr//DTD IUCr article dtd V1.1//EN"><?show "^totalfigures"3><?show "^totaltables"2><?show "^totalschemes"0><?Pub Inc><iucr-art epubday="06" epubmo="07" epubyr="2011" language="0" docsubty="fa" pii="S0108767311020137" aid="sc5042" access="pay" version="1.1.0" jid="a112013" crt="International Union of Crystallography"><jnlinfo issn="0108-7673" coden="ACACEQ" fpage="430" subtitle="Foundations of Crystallography" name="Acta Crystallographica Section A" abbrtitle="Acta Cryst. A" yr="2011" volume="67" doi="10.1107/S0108767311020137" editor="D. Schwarzenbach" lpage="434" partno="00" issue="05"><fm><atl>Direct methods: a paradox with regard to the convergence of random phase trials toward <?show [forcelb]>solutions</atl><shortatl>Direct methods</shortatl><aug><au><fnm inits="D.A.">D. A.</fnm><snm index="Langs, D.A.">Langs</snm></au><orf id="a"><cor contact="yes" correspondence="yes" email="langs@hwi.buffalo.edu"><!-- comment --></cor><au><fnm inits="H.A.">H. A.</fnm><snm index="Hauptman, H.A.">Hauptman</snm></au><orf id="a"><aff><oid id="a"><department>Department of Structural Biology</department>, <organisation>Hauptman–Woodward Medical Research Institute</organisation>, <street>700 Ellicott Street</street>, <cty>Buffalo</cty>, NY <postcode>14203</postcode>, <cny cny-code="us">USA</cny></aff></aug><shortaug>Langs and Hauptman</shortaug><re yr="2011" mo="03" day="03"><acc yr="2011" mo="05" day="26"><synopsis> A large variance in the 'shake-and-bake' minimized target function <it>R</it>(ϕ<inf arrange="stagger">h</inf>) can identify large subsets of phases whose mean phase error is considerably smaller than the average during unsuccessful phasing trials when the overall phase error occasionally dips below 75 or 80°. Efforts to exploit this observation to promote convergence to the solution, however, are generally not successful. </synopsis><abs> A frustrating observation, based on an <it>R</it><inf arrange="stagger">min</inf> variance analysis within the 'shake and bake' framework of direct methods phasing, is described. The variance of <it>R</it><inf arrange="stagger">min</inf> can on occasion identify large subsets of phases that have a significantly lower mean phase error than the entire direct methods phase set of otherwise unsuccessful phasing trials for which the overall phase error occasionally dips below 75 or 80°. This is the first time, other than for a handful of Σ1 phase indications in optimal situations, that <it>a priori</it> phase estimates have been attained for large numbers of <it>E</it> values, prior to solving the structure. Although the <it>a priori</it> variance of <it>R</it><inf arrange="stagger">min</inf> is a useful tool for identifying such phases, the <it>a posteriori</it> phase refinement shifts indicated by its minimum often prevent a successful convergence to the solution. Similar efforts to encourage solution convergences in the realm of real space have also been discouraging. </abs><kwdg><kwd>random phase trials</kwd><kwd>variance analysis</kwd><kwd>direct phasing methods</kwd><kwd>'shake and bake' phasing procedure</kwd></kwdg></fm><bdy><sec id="sec1"><st>Introduction</st> <?tpt=-12pt><qd> 'How wonderful that we have met with a paradox. Now we have some hope of making progress.' (Niels Bohr) </qd> The shake-and-bake (SnB) direct methods phasing procedure (Hauptman, 1988<bbr id="bb3">; DeTitta <it>et al.</it>, 1994<bbr id="bb1">; Weeks <it>et al.</it>, 1994<bbr id="bb15">) has provided a significant improvement over older direct methods phasing procedures based on the tangent formula

94% | ISO | R 429 <431> 434 | /a/sc5042/sc5042.3d – changed | 15:37:07

Checks and changes made in editing

- Authors and affiliations are correct
- Abstract not written in first person
- Spelling
- Correction of grammar
- Clarity/avoidance of ambiguity
- Hyphenation: adjectival phrases, *e.g.* electron-density plot, en rules used to link connected items *e.g.* pump–probe experiment
- Consistency between text and tables/figures, especially labels
- Arrangement of data in tables, economic presentation
- Figure quality, clarity, size, labels and layout
- Use of abbreviations
- References complete and in correct style

Crystallography Journals Online

Checks and changes made in editing (continued)

- Nomenclature is correct
- Units are SI
- Special symbols (Greek, maths) are correct
- Tables, figures, schemes are numbered in the order they are mentioned in the text
- Equations numbered sequentially
- Check required data have been deposited in databases
- Supplementary material (not edited) is in the correct format for archiving
- Add appropriate links to structural databases *etc.*
- **Any queries appear as bold and underlined in the proofs**

Crystallography Journals Online

Proofs and corrections

- Low-resolution pdf proofs with order form sent to contact author
- Corrections (preferably received as an email: line number, correction) are made
- Article is proofread one last time
- Final page make-up: line breaks, no widows/orphans, figures and tables are near relevant text (if possible)
- Final PostScript (for online pdfs and for printing)
- Paper details added to the 'issue instance'

Crystallography Journals Online