

Re: Taxol: molfile Date: Fri, 1 Jan 93 24:11:05 EST From: Francl Michelle M <mf@mcm.brynmavr.edu> Date: 6 Jan 1993 10:55:29 -0500 (EST) From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON, DOUGLAS_W@LILLY.COM> Subject: u
kfz-heidelberg.de>Subject: energy contribution of hbonds?Date: 06 Jan 1993 10:55:29 -0500 (EST) From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON, DOUGLAS_W@LILLY.COM> Subject: u
: CADD videosDate: wed, 6 Jan 93 13:03:33 -0800From: chiremv@andromeda.jeffb@uunet.UU.NET (Jeff Blaney) Subject: Re: Polygon-based solvent accessible surfacesDate: Thu, 7 Jan 93
!!Date: 08 Jan 1993 09:19:39 -0500 (EST) From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON, DOUGLAS_W@LILLY.COM> Subject: replies to my posting about PDB searching methodsDate: F
vi@tiberius.tc.cornell.edu>From: scsupham@reading.ac.ukDate: Mon, 11 Jan 93 17:54:05 GMT Subject: DMol questionsDate: Mon, 11 Jan 1993 14:33 EST From: WILLIAMS%XRAY2@ulkyvx02.loui
or doubled messagesDate: wed, 13 Jan 93 13:38:09 EST From: rsefeck@watson.ibm.com Subject: data-flow programs for molecular modelingDate: wed, 13 Jan 93 13:38:09 EST From: rsefeck@
GAMESS and MOPACDate: Thu, 14 Jan 1993 10:42:35 -0500 (EST) From: HERMAN@ULNA.BWH.HARVARD.EDU Subject: RE: HELPDate: Thu, 14 Jan 1993 11:18:26 -0500 From: jle@world.std.com (Joe
Gaw (Ron Shepard) Subject: Re: Cartesian vs Internal coordinatesDate: Fri, 15 Jan 93 06:48 CDT From: CUNDARIT@MEMSTVX1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU Subject: Steric strain at T
0From: dmschn@bbt.monsanto.com Subject: next Molecular Graphics Society MeetingFrom: m.e. <harbowy@chemres.tn.cornell.edu> Subject: UHF calc's on diradicals/TSDate: Mon, 18 Jan 9
n 93 15:29:22 +0100 From: oosten@rulhml.LeidenUniv.nl (A.B. van Oosten) Subject: Re: proton+electron+neutron?Date: wed, 20 Jan 93 10:11:36 EST From: landman@hal.physics.wayne.edu
O-STATE.EDU>Subject: RE: PC Survey RESULTSDate: wed, 20 Jan 1993 15:47 CST From: "JORGE M. SEMINARIO" <JSMCM@royal.crc.uno.edu> Subject: Re: density problemDate: wed, 20 Jan 93
ke to test a program.Date: Thu, 21 Jan 93 12:19:42 +0100 From: Inst.f. Phys.Chem. I <pci@pctc.chemie.uni-erlangen.de> Date: 21 Jan 93 07:50:00 EST From: nauss@wrair-emh1.army.mil SU
Jan 93 13:27:12 GMT From: "D. Mathieu" <DEWINDT@FRSAC11.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU> Subject: force constant symmetry and Gaussian90Date: 22 Jan 93 13:06:32 UTF From: "BD
le RecurrenceDate: Fri, 22 Jan 1993 13:36:26 +0000 From: BDIEAL <BDIEAL@camsci.com> Subject: RE: PDB on the MacDate: Thu, 21 Jan 93 17:31:46 -0500 From: system@alchemy.chem.utoron
From: arne@mango.mef.ki.se (Arne Elofsson) Subject: Re: charmm and SGIs - charmm newsgroup?Date: Sun, 24 Jan 93 15:05:30 -0500 From: chm_ramsay@emunix.emich.edu Subject: CHEMICALC:
Subject: This is testDate: 26 Jan 93 00:20:33 -0600 (CST) From: "NOLPER@VAX1.UMCK.EDU" <nolper@vax1.umck.edu> Subject: Re: density problemDate: Thu, 21 Jan 93 12:57:08 -0500 From: watanabe@tammy.ha
ate: 27 Jan 93 08:59:32-0500 From: "N-D" <D.W.ROD@DD.IDEAS.COM> Subject: Re: density problemDate: Thu, 21 Jan 93 12:57:08 -0500 From: watanabe@tammy.ha
3 20:38:08 GMT Subject: Re: XWD->Mac conversion?Date: wed, 27 Jan 93 15:21:29 -0700 From: "JUN KUSNO" <jkusno@chem.uci.edu> Subject: Re: Periodic Table WidgetDate: wed, 27
93 14:47:36 -0500 From: caves@tammy.harvard.edu Date: Thu, 28 Jan 1993 15:28:31 PST From: VOODOO CHILE <morris@gn12.ucdavis.edu> Subject: Population Analysis in GaussianFrom: mei@ve
1993 14:23:55 +22305823 (EST) Date: Fri, 29 Jan 93 15:07:15 PST From: Ron Shepard <hrac@csail.mit.edu> Subject: Periodic Table WidgetDate: Fri, 29 Jan 1993 16:47:38 -0600 From: sliu
CHEM.CMU.EDU Subject: RE: Gaussian and excited statesDate: Fri, 29 Jan 93 15:07:15 PST From: Ron Shepard <hrac@csail.mit.edu> Subject: Periodic Table WidgetDate: Fri, 29 Jan 93 15
radomski@mond1.ccr.c.uga.edu Date: Mon, 1 Feb 1993 12:34:28 +0500 From: "FALLOU" <falou@usermail.uni-stuttgart.de> Subject: Cerebral AnnouncementDate: 01 Feb 93 19:26:49-0500 From: SBPM
: youkha@biosym.com Subject: Summary: Internals & Non-BondsDate: Tue, 2 Feb 93 11:12:51 CST From: (baell) <baell@syd.dah.csiro.au> Subject: DMF dielectricDate: Mon, 1 Feb 93 17:57
un.nl> Subject: Electronic Periodic TablesDate: 02 Feb 1993 14:36:03 -0500 (EST) From: ZURAW@athena.leia.polaroid.com Subject: 3D structure -> 2D drawing? From: QINGSONG@minmet.lan.
and NanotechnologiesDate: wed, 3 Feb 93 10:46:20 MST From: QINGSONG@minmet.lan.mcgill.ca Date: 3 Feb 93 13:04:57 Subject: software for calculating zeta potential and e
OF TOLEDO" <DSMITH@uoft02.utoledo.edu> Subject: Re: Plotting Orbitals from a G90/G92 CalculationDate: Thu, 4 Feb 93 11:27:53 EST From: Kevin Moore <kmoore@ncsc.org> Subject: MOLSOL
3 +0100 (NFT) Date: 05 Feb 93 09:28:33 EST From: Elliot King <71127.1231@compuserve.com> Subject: Call for PapersDate: Fri, 5 Feb 1993 16:17:32 +0100 From: ivan@gandalf.ciam.unibo.i
<bobby_clark@quickmail.clemson.edu> Subject: E-mail searchDate: 6 Feb 1993 10:08:20 -1812 From: "Bobby Clark" <bobby_clark@quickmail.clemson.edu> Subject: Memory and CPU for Starde
500 (EST) From: spollack@ester.mse.uc.edu (S.K. Pollack) Subject: Phosphazene ModelingDate: Mon, 8 Feb 93 07:58:51 EST From: adit@kodak.COM (Adi Treasurywala) Subject: Coordinates o
Date: Tue, 09 Feb 1993 21:39:58 -0500 (EST) From: "DR. DOUGLAS A. SMITH, UNIVERSITY OF TOLEDO" <DSMITH@uoft02.utoledo.edu> Subject: parallel workstations and serversDate: wed, 10
S.From: Zhou Feng <feng@lisboa.ks.uiuc.edu> Date: wed, 10 Feb 93 16:23:41 -0600 Subject: parallel CHARMM?Date: wed, 10 Feb 93 15:46:43 -0800 From: rickl@biosym.com Subject: DIBUG a
-2 Subject: Re: ZINDO programDate: 11 Feb 1993 13:06:18 +0100 From: schettler@chemix.mpi-stuttgart.mpg.de Subject: Mac summeryFrom: theresa@si.fi.ameslab.gov (Theresa Windus) S
/14031%hkuxa.hku.hk@OHSTVMA.ACS.OHIO-STATE.EDU Subject: MO Plotting program!Date: Fri, 12 Feb 93 09:48:41 CET From: Norbert Mueller <K360171%EDVZ.UNI-Linz.AC.%@OHSTVMA.ACS
t: Re: X windows for PC ..Date: Sat, 13 Feb 93 12:44:490000 From: Katsuhiko Kobayashi <kobayashi@chem.tokai.ac.jp> Subject: X windows for PC ..Date: Sat, 13 Feb 1993 14:47:09 +0100 (WET) From: PREINERT@biolan.u
ell.edu> Subject: MPW Fortran?Date: Tue, 16 Feb 93 11:29:01 PST From: "w. Todd wipke" <wipke@SECS.UCSC.EDU> Subject: Final Call Summer Undergraduate Research Fellowship (SURF)Date: wed, 17 Feb 1993 14:15:16 -0500 (EST) From: "DR. DOUGLAS A. S
Thu, 18 Feb 93 14:22:08 PST From: raw@autodesk.com (Robert A. Whiteside) Subject: Re: Question about PDB formatDate: Thu, 18 Feb 93 14:02:32 PST From: fisher@scripps.edu (Cindy Fiske
feld chargesDate: Fri, 19 Feb 93 14:49:00 PST From: "DR. DOUGLAS A. SMITH, UNIVERSITY OF TOLEDO" <DSMITH@uoft02.utoledo.edu> Subject: parallel workstations and serversDate: wed, 10
k Kjemi" <bjerkese@kjemi.unit.no> Subject: Summary: Scaled Freq for S and HDate: Sun, 21 Feb 1993 20:51:19 +0100 (MET) Subject: Long Time-scale DynamicsDate: Mon, 22 Feb 93 16:49:
: Carl JugDate: Tue, 23 Feb 93 15:08:43 PST From: wsonnen@alnitak.usc.edu (Wayne Sonnen) Subject: dna base chargesDate: 23 Feb 93 15:38:36-2300 From: "Alexandre MICU P16A" <alex@ba
g) Subject: Re: Hydrogen bond.Date: wed, 24 Feb 93 17:21 EDT From: <PODOSNNA%NYUACF1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU> Subject: X-window terminal emulator for MacDate: Thu,
nl.gov Subject: X-window terminal emulator for MacDate: Thu, 25 Feb 93 17:19:09 -0500 From: feng@soi.chem.temple.edu (Feng Chen) Subject: X-windows Server on MS-WindowsDate: Thu, 2
d.harvard.edu (jill) Subject: Re: Question about PDB formatDate: Thu, 18 Feb 93 14:02:32 PST From: fisher@scripps.edu (Cindy Fiske) Subject: language questi
semiempirical calculations Simple oxidations: Sender@chemdcl.tau.ac.il (Sender@chemdcl.tau.ac.il) Subject: MOPACDate: Sun, 20 Feb 93 13:44:41 GMT Date: Mon, 1 Mar 1993 15:25:19
n.de Subject: Expert Know-How wanted !!Date: 02 Mar 1993 08:48 -0500 (EST) From: "RONALD B. WILSON" <ROYALD@LILLY.COM> Subject: new book on computational chemistryDate: Tue
ate.Edu (Gene Carter) Subject: Co MD parameters.Date: Tue, 23 Feb 1993 12:55 EST From: "RONALD B. WILSON" <ROYALD@LILLY.COM> Subject: new book on computational chemistryDate: Tue
lling Software: Does anyone have STELLA?Date: 04 Mar 1993 17:08:31 -0500 (EST) From: MARYJO@northeastern.edu Subject: PDB subdir organization? From: Jan Labanowski <jkl@cc1.net> Dat
ar 93 17:30:16 GMT Date: Sun, 7 Mar 93 12:36 EST From: <SML108@PSUVM.PSU.EDU> Subject: Minimum allowable interatomic separationsFrom: sender@chemdcl.tau.ac.il (Senderowitz Hanoc
succ.f.cnr.it Subject: MO Theory Made VisibleDate: Tue Mar 09 11:23:12 1993Date: Tue, 9 Mar 93 10:52:25 -0500 From: gallion@auriga.rose.brandeis.edu (steve gallion) Subject: GRO
upliffeDate: Thu, 11 Mar 93 18:54 EDT From: <PODOSNNA%NYUACF1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU> Subject: Software for PCDate: Fri, 12 Mar 93 04:51:15 GMT From: jim@quanta.phy.
r 1993 02:33:09 -0800 (PST) From: Thomas Nhan <tom@cassandra.cornell.edu> Subject: Re: Question about PDB formatDate: Sun, 14 Mar 93 11:06:13 +0100 From: doelz@comp.bioz.unibas.ch (Re
MA.ACS.OHIO-STATE.EDU> Subject: partial charges for fictive atomsDate: Mon, 15 Mar 1993 12:55:05 -0600 (CST) From: Chris Parkinson <mbdtscp@hpc.ch.man.ac.uk> Subject: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMT Subject: Re: MM2 code for UN
ar 1993 13:58:26 -0400 From: ZSHI@ac.dal.ca Subject: Information about IBM RS6000Date: 17 Mar 93 16:18:00 EDT From: "STEPHEN R. HELLER" <srheller@asr.arsusda.gov> Subject: Software
st Girona seminar on Molecular SimilarityDate: Thu, 18 Mar 93 10:40:05 CET From: ZSYAMP01@EBCECS@OHSTVMA.ACS.OHIO-STATE.EDU Subject: First Congress of the ISTCP (pa
:11 -0500 Subject: Keep the noise down, pleaseDate: 19 Mar 93 11:37:00 EST From: nauss@wrair-emh1.army.mil Subject: Program called GRIDDate: Fri, 19 Mar 93 14:33:18 EST From: Ge
23 -0600 (CST) From: Andy Holder <AHOLDER@VAX1.UMCK.EDU> Subject: Announcing AMPAC 4.5Date: 21 Mar 1993 17:36:57 -0600 (CST) From: Andy Holder <AHOLDER@VAX1.UMCK.EDU> Subject: Semic
.mil Subject: what about simulated annealing?Date: wed, 24 Mar 93 14:11:32 +0100 From: dufner@ws01.pc.chemie.th-darmstadt.de (Hagen Dufner) Subject: efg in g92From: "Christopher J
ject: 5C&A Conference speakers - thanksDate: Thu, 25 Mar 93 10:18:48 -0500 From: au195@cleveland.freenet.edu (Dr. Gene A. Nelson) Subject: Batching files in MOPACFrom: zrf10128@w
DICH1.UNINA.IT Subject: looking for ACES programFrom: Robert Laird <mbdtsrl@hpb.ch.man.ac.uk> Subject: Fe-o calculationDate: Mon, 29 Mar 93 15:49:03 BST From: rafapa@obel
: Polyrate queryDate: Tue, 30 Mar 1993 19:31:32 +0200 From: c62@aixfile1.urz.uni-heidelberg.de (Andreas Schulz) Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 -
t: Stephen R. WilsonDate: Thu, 1 Apr 1993 16:33:29 +0200 From: oles@gollum.uio.no Subject: BiosymDate: 01 Apr 1993 11:43:13 -0600 (CST) From: CUNDARIT@memstvx1.memst.edu

CCLE: une « mailing list » en tant que corpus.

Alexandre Hocquet
Université de Lorraine & CAK

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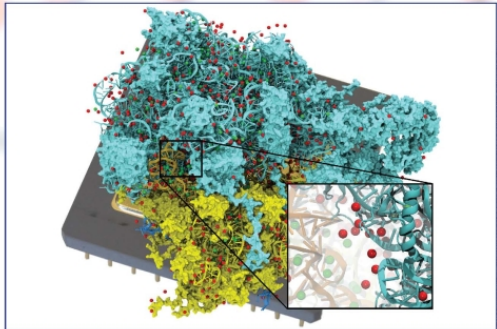


Subject: Re: Taxol
Date: Fri, 14 Jan 1993 14:11:05
Subject: energy contribution of bonds
Date: 06 Jan 1993 10:55:29 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: u
emv!andromeda!jeffb@uunet.UU.NET (Jeff Blaney)Subject: Re: Polygon-based solvent accessible surfacesDate: Thu, 7 Jan 93
com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: replies to my posting about PDB searching methodsDate: F
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(EST)From: HERMAN@ULNA.BWH.HARVARD.EDUSubject: RE:HELPPDate: Thu, 14 Jan 1993 11:18:26 -0500From: jle@world.std.com (Joe
inatesDate: Fri, 15 Jan 93 06:48 CSTFrom: CUNDAKIT@MEMSTVX1.BTNET@OHSTVMA.ACS.OHIO-STATE.EDUSubject: steric strain
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Subject: Re:CACHE on the MacDate: Tue, 2 Mar 9
Date: Tue, 2 Mar 9
Subject: Software for PCDate: Fri, 12 Mar 93 04:51:15 GMTFrom: jim@quanta.phy.
Date: Sun, 14 Mar 93 11:06:13 +0100From: doelz@comp.bioz.unibas.ch (Re
Date: Tue, 16 Mar 93 11:49:43 GMTSubject: Re: MM2 code for UN
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Date: Thu, 1 Apr 1993 16:33:29 +0200From: oles@gollum.uio.noSubject: BiosynDate: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNDAKIT@memstvx1.memst.edu

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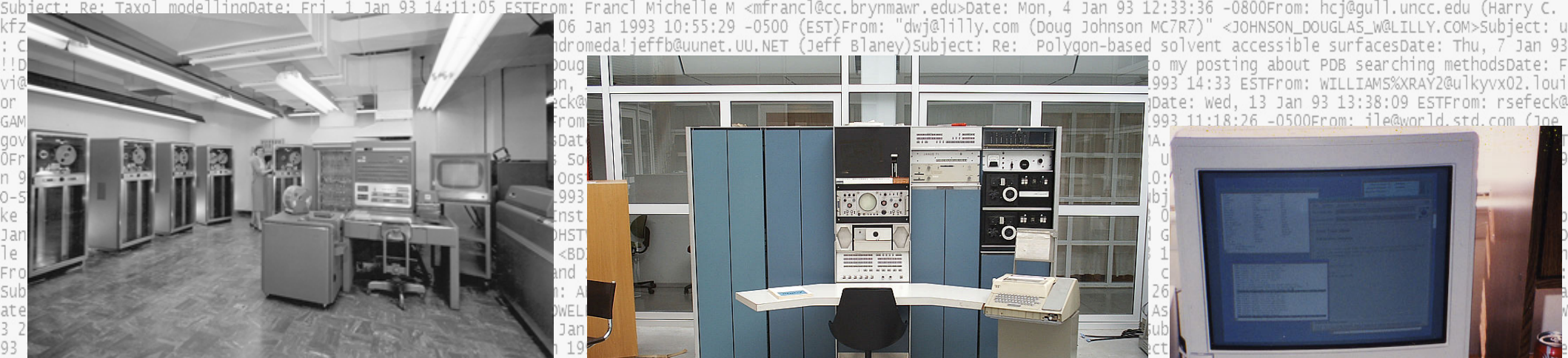


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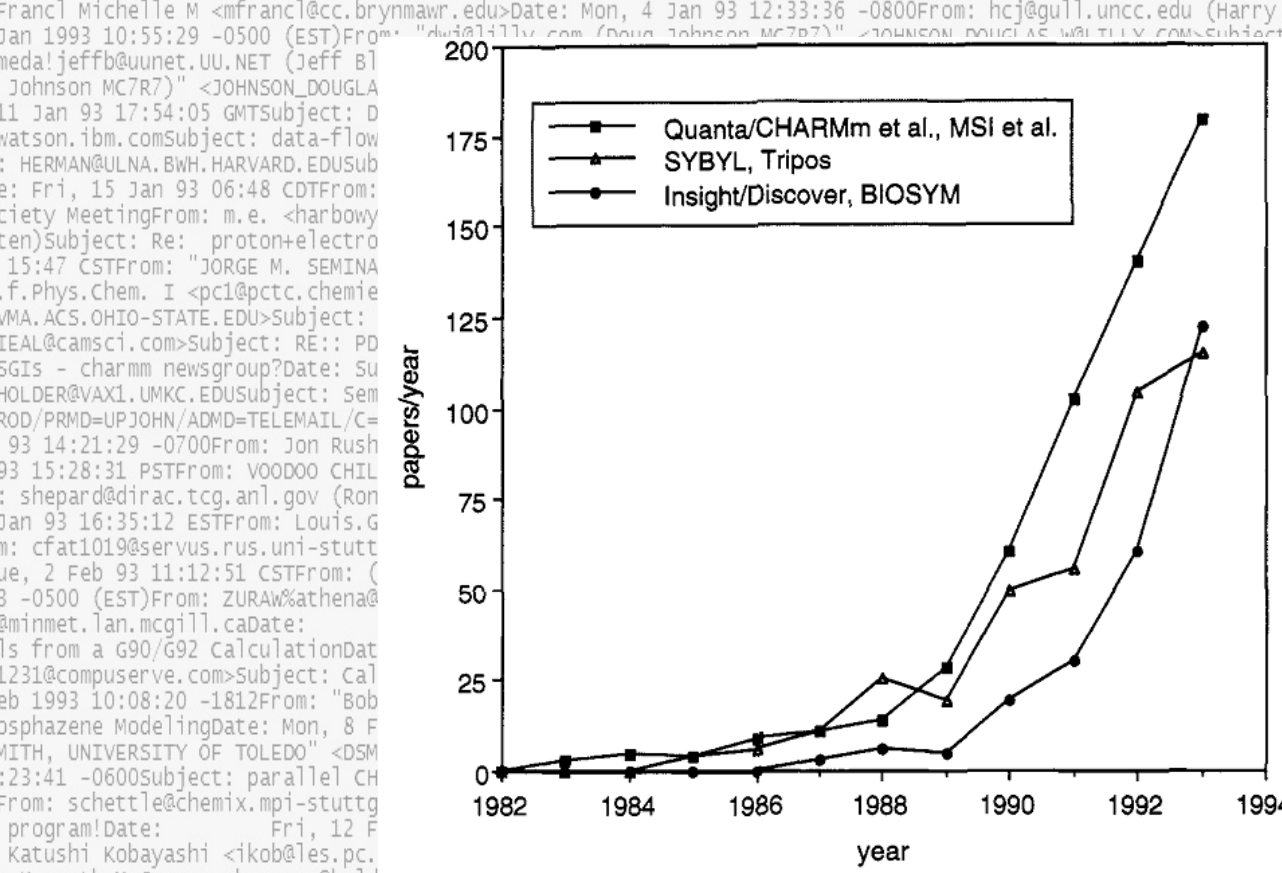
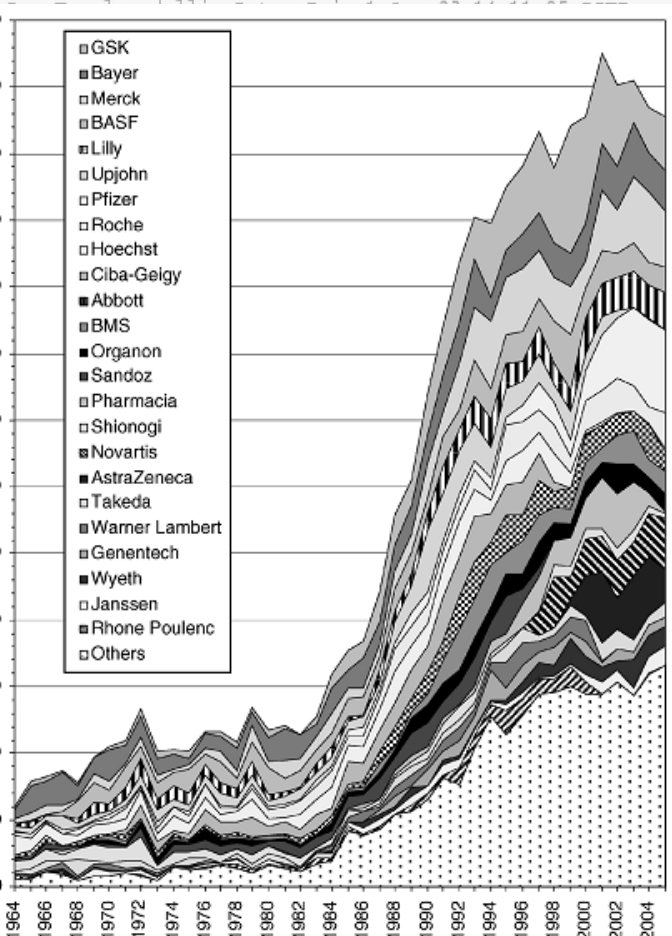
Supercomputers -> Graphic terminals, Personal Computers

Developer et User ne sont plus la même personne: que faire

du logiciel?

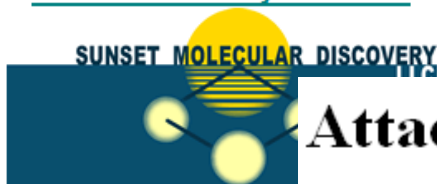
Communauté scientifique différente de la « république des

informaticiens » (Flichy)



Constructeurs d'ordinateurs → Industrie pharmaceutique

Software : Publier? Vendre? Partager? Code Source?



Attack of the killer workstations

<http://www.ccl.net/ind>

CCL Home

Messages in a queue: 0 (approx. wait time: 00:0

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Welcome to the CCL Website!

ACS COMP Division supports CCL:

- From: jle@world.std.com (Joe M Leonard)
- Subject: Attack of the killer workstations
- Date: Tue, 10 Dec 91 20:04:44 -0500

Reviewing the recent discussion regarding C vs. Fortran and structured vs. spaghetti coding, isn't it reasonable to consider the time of the programmer as more important than the code's runtime (within reason)? Given that approx. \$20k workstations are comparable to Cray machines, isn't 10-ish% overhead more than worth the human time savings through better-thought-out programming (structured, modular, OO, etc.)? I hope the day's past for really needing to count cycles in loops - as one can wait for the next version of workstation xxx to gain appreciable speedups. Obviously, this isn't the case for mpp machines, for which the consensus is that one must rethink and/or reimplement algorithm's in order to use the hardware to advantage. Still, this might prove to be an example where clearer coding styles might turn out to be a win after all...

Joe Leonard

jle@world.std.com

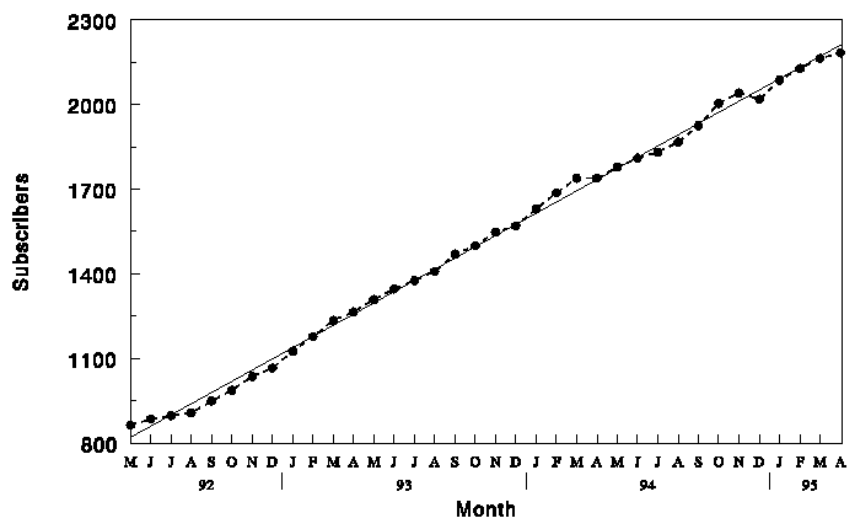
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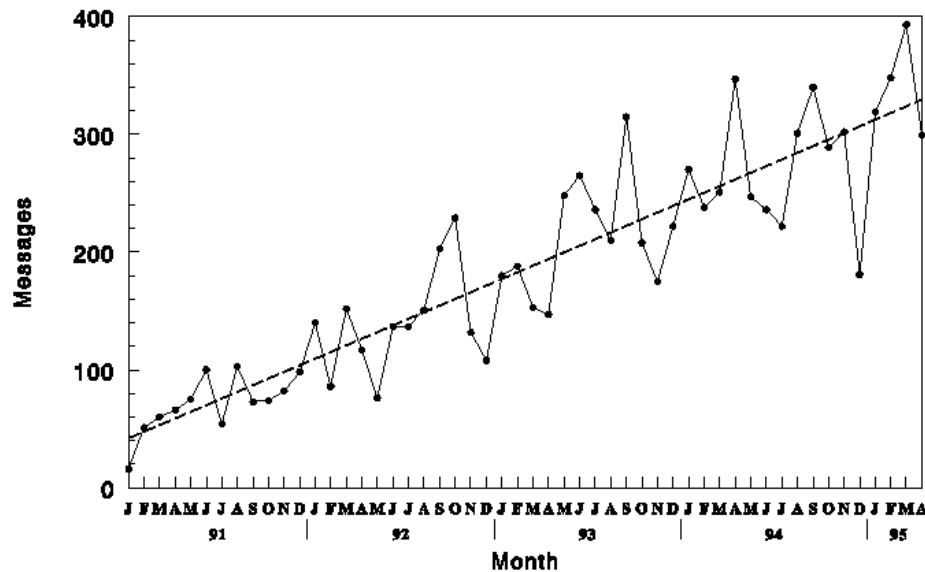
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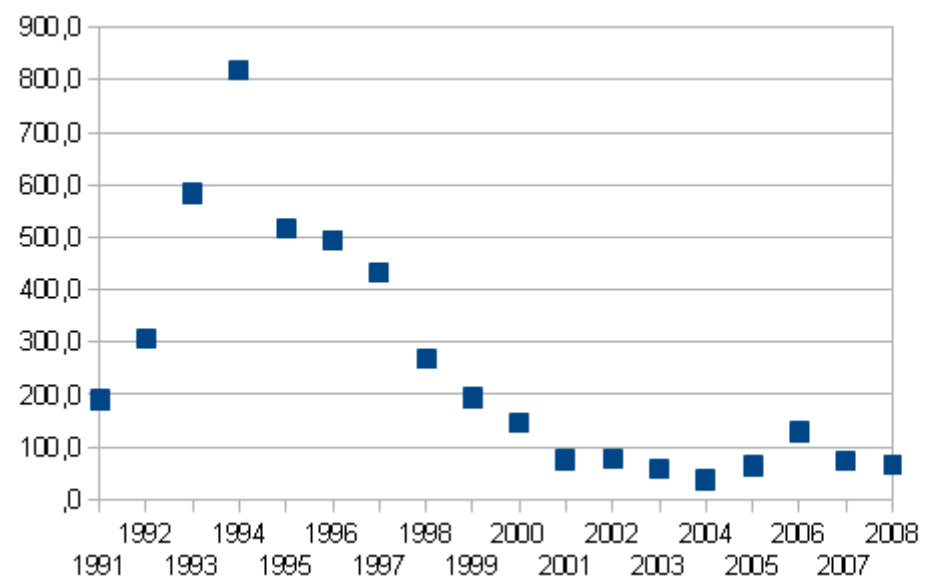


Messages per month



-croissance régulière puis stabilisation (approx. 10 messages par jour) : succès = équilibre entre attrition et explosion.

Subject: Re: Taxol modellingDate: Fri, 1 Jan 93 14:11:05 ESTFrom: Fran1 Michelle M <mfran1@cc.brynmawr.edu>Subject: u
kfz-heidelberg.de>Subject: energy contribution of hbonds?Date: 06 Jan 1993 10:55:29 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON.DOUGLAS_W@LILLY.COM>Subject: u
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Text mining ; temporel

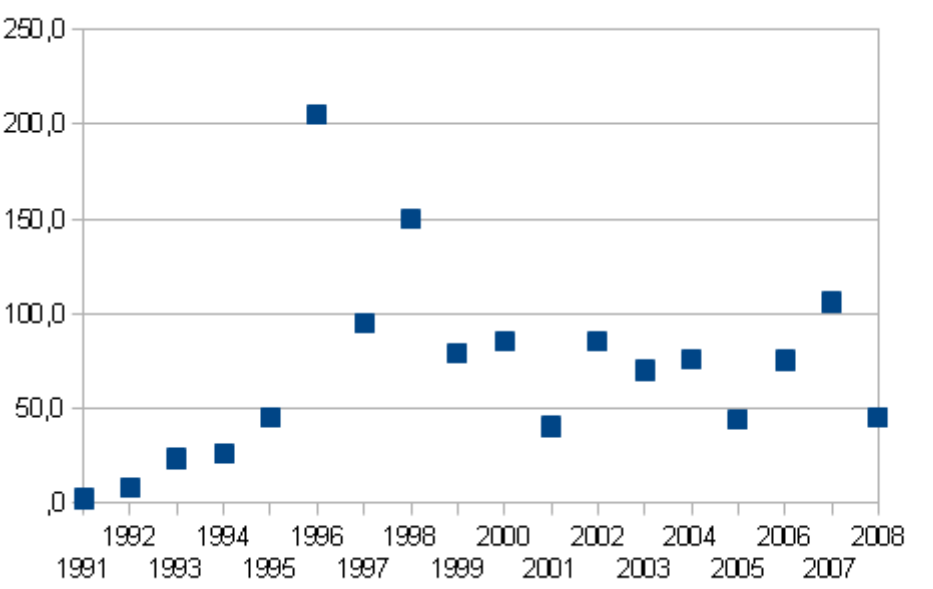
Occurrences du mot

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500 (EST)From: spoilack@ester.mse.uc.EDU (S.K. Pollack)Subject: Phosphazene ModelingDate: Mon, 8 Feb 93 07:58:51 ESTFrom: adit@kodak.COM (Adi Treasurywala)Subject: Coordinates o
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/14031@hkuxa.hku.hk@OHSTVMA.ACS.OHIO-STATE.EDUSubject: MO Plotting program!Date: Fri, 12 Feb 93 09:48:41 CETFrom: Norbert Mueller <360171%EDVZ.UNI-Linz.AC.%@OHSTVMA.ACS
t: Re: X Windows for PC ..Date: Sat, 13 Feb 93 12:21:47 +0900From: Katushi Kobavashi <ikob@les.ac.uec.ac.jp>Subject: Re: X Windows for PC ..Date: Tue, 16 Feb 93 11:29:01 PS

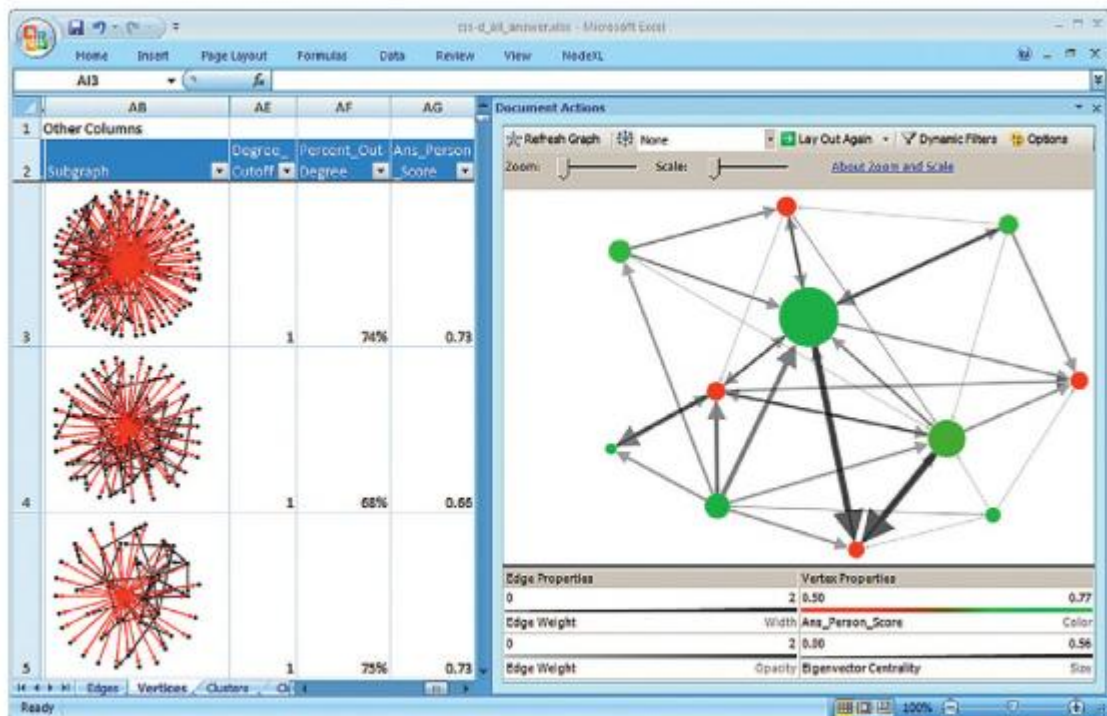
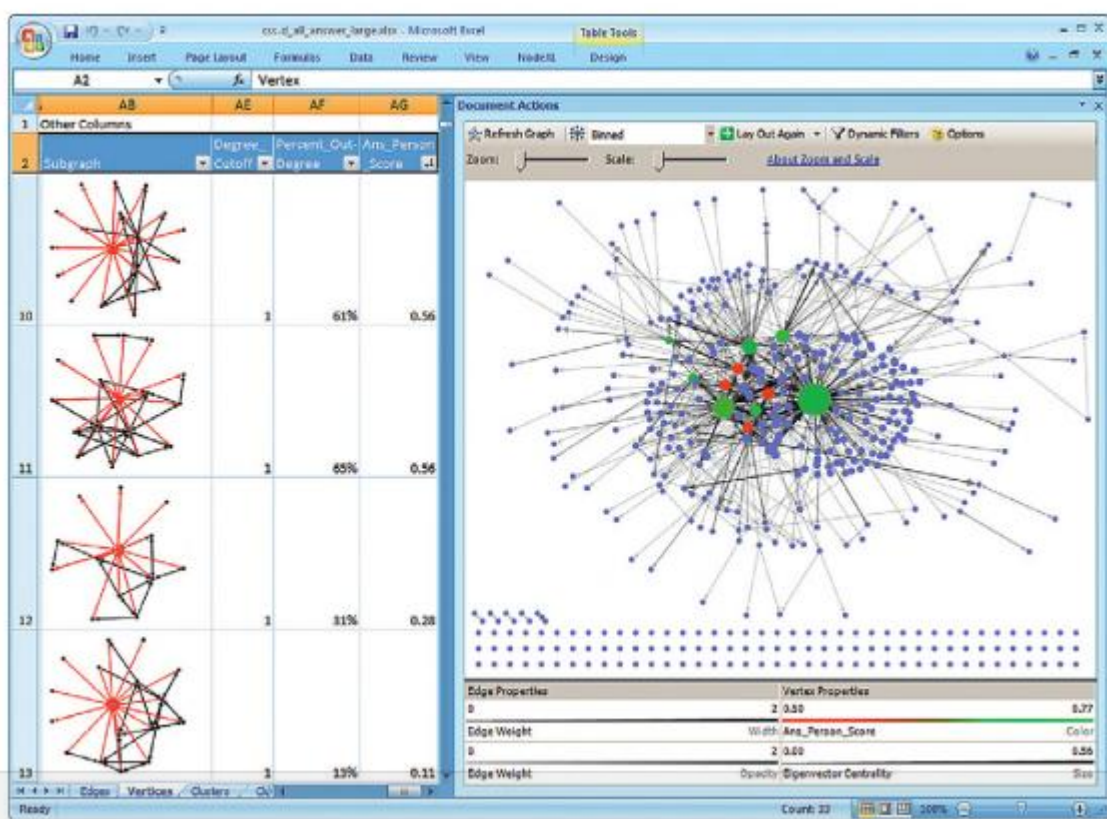
Occurrences du mot

« freeware »



MO@CHEMNA.DICHI.UNINA.ITSubject: looking for ACES programFrom: Robert Laird <mboatsr@npp.cn.man.ac.uk>Subject: Polyrate QueryDate: Tue, 30 Mar 1993 19:31:32 +0200From: c62@aixfile1.urz.uni-heidelberg.de (Andreas Schulz)Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 -
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awr.edu: Mon, 6 Jan 93 12:33:36 -0800From: hcj@gull1.uncc.edu (Harry C. "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON.DOUGLAS_W@LILLY.COM>Subject: u
y)Subject: Re: Polygon-based solvent accessible surfacesDate: Thu, 7 Jan 93
@LILLY.COM>Subject: replies to my posting about PDB searching methodsDate: F
questionsDate: Fri, 93 14:33 ESTFrom: WILLIAMS%XRAY2@ulkyvxo2.loui
ograms for molecular modelingDate: wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@
t: RE:HELPDate: Thu, 14 Jan 1993 11:18:26 -0500From: jle@world.std.com (Joe
NDARIT@MEMSTVX1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>Subject: Steric strain at T
emres.milsubj: Date: Mon, 18 Jan 9
eutron?Date: wed, 20 Jan 93 10:11:36 ESTFrom: landman@hal.physics.wayne.edu
<JSMCM@royal.crc.uno.edu>Subject: Re: density problemDate: wed, 20 Jan 93
i-erlan...Date: 93 03 14 10:59:00 From: wvair-emh1.army.milSU
force...Date: 93 03 14 10:59:00 From: wvair-emh1.army.milSU
n the MacDate: Thu, 21 Jan 93 17:31:46 -0500From: system@alchemy.chem.utoron
24 Jan 93 15:05:30 -0500From: chm_ramsay@emunix.emich.eduSubject: CHEMICALC:
pirical...Date: 93 03 14 10:59:00 From: wvair-emh1.army.milSU
@sprint.com>Subject: Computer Assisted Chemistry Course Info RequestedDate: 27
rusho@nitrate.chem.utah.edu>Subject: Re: Periodic Table WidgetDate: wed, 27
moris@gnl2.ucdavis.edu>Subject: Population Analysis in GaussianFrom: mei@ve
epard)S...Date: 93 03 14 10:59:00 From: wvair-emh1.army.milSU
e@um.cc.umich.edu>Subject: Gaussian and excited statesDate: Fri, 29 Jan 93 15
t.de>Subject: Conference AnnouncementDate: 01 Feb 93 19:26:49-0500From: SBPM
11) <baello@dab.csirugau>Subject: DMF dielectric Date: Mon, 1 Feb 93 17:57
a.polar...Date: 93 03 14 10:59:00 From: wvair-emh1.army.milSU
From: QINGSONG@minmet.lan.
3 Feb 93 13:04:57>Subject: software for calculating zeta potential and e
Thu, 4 Feb 93 11:27:53 ESTFrom: Kevin Moore <kmoore@ncsc.org>Subject: MOLSOL
or PaperDate: Fri, 5 Feb 1993 16:17:32 +0100From: ivan@gandalf.ciam.unibo.i
Clark" <clark@lilly.com>Subject: Memory and CPU for Starde
93 07:58:51 ESTFrom: adit@kodak.COM (Adi Treasurywala)Subject: Coordinates o
@uoft02.utoledo.edu>Subject: parallel workstations and serversDate: wed, 10
M?Date: wed, 10 Feb 93 15:46:43 -0800From: rickl@biosym.comSubject: DIBUG ad
.mpg.de>Subject: Mac summeryFrom: theresa@si.fi.ameslab.gov (Theresa Windus)S
93 09:48:41 CETFrom: Norbert Mueller <K360171%EDVZ.UNI-Linz.AC.%@OHSTVMA.ACS
.ac.jp>Date: Sat, 13 Feb 1993 14:47:09 +0100 (WET)From: PREINERT@biolan.u
.sid.h...>Subject: Re: X windows for PC ..Date: Tue, 16 Feb 93 11:29:01 PS
hip (SURF)Date: wed, 17 Feb 1993 14:15:16 -0500 (EST)From: "DR. DOUGLAS A. S
formatDate: Thu, 18 Feb 93 17:02:32 PSTFrom: fisher@scripps.edu (Cindy Fische
SSE calculationDate: Fri, 19 Feb 93 11:53:05 -0500From: G. Ravishanker <ravi
1:19 +0100 (MET)Subject: Long Time-scale DynamicsDate: Mon, 22 Feb 93 16:49:
ase chargesDate: 23 Feb 93 15:38:36-2300From: "Alexandre MICU P16A" <alex@ba
A.ACS.OHIO-STATE.EDU>Subject: X-window terminal emulator for MacDate: Thu,
em.temple...>Subject: X-windows Server on MS-windowsDate: Thu, 7
Feb 1993 15:00:00 From: swang@kjemi.uio.no>Subject: language questi
PAC6.0Date: sun, 28 Feb 93 13:44:41 GMT-2:00Date: Mon, 1 Mar 1993 15:25:19
OYD_DONALD_B@LILLY.COM>Subject: new book on computational chemistryDate: Tue
andrum...>Subject: Re:Cache on the MacDate: Tue, 2 Mar 9
rn.edu>Subject: PDB subunit organizationFrom: Jan Labanowski <jkl@cc1.net>Dat
ble interatomic separationsFrom: sender@chemdcl.tau.ac.il (Senderowitz Hanoc
25 -0500From: gallion@auriga.rose.brandeis.edu (steve gallion)Subject: GRO
ject: Fe-O for...Date: Mar 93 04:51:15 GMTFrom: jim@quanta.phy.
ile...Date: sun, 14 Mar 93 11:06:13 +0100From: doelz@comp.bioz.unibas.ch (Re
STFrom: HSUS@chemv2.mps.ohio-state.edu>Subject: Problem with vibrational freq
or UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UN
00 EDT...>Subject: "LILLY" <srheller@asrn.arsusda.gov>Subject: Software
SCA1@OHSTVMA.ACS.OHIO-STATE.EDU>Subject: First Congress of the ISTCP (pa
mils>Subject: Program called GRIDDate: Fri, 19 Mar 93 14:33:18 ESTFrom: Ge
17:36:57 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Semic
hemie.th-darmstadt.de (Hagen Dufner)Subject: efg in g92From: "Christopher J
et.edu (Dr. Gene A. Nelson)Subject: Batching files in MOPACFrom: zrf10128@a
>Subject: Fe-o calculationDate: Mon, 29 Mar 93 15:49:03 BSTFrom: rafapa@obel
de (Andreas Schulz)Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 -
osymDate: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNDARIT@memstvx1.memst.edu

Threaded
Conversation Social
Network Analysis:
-reply network
-user to user network
-thread to thread
network

-Rôles des intervenants
-Hot Topics (Hansen)

IEEE Annals

A Social History of Bitnet and Listserv, 1985-1991

April-June 2000 (vol. 22 no. 2)

pp. 32-41

David Alan Grier

Mary Campbell

DOI Bookmark: <http://doi.ieeeecomputersociety.org/10.1109/85.841135>

ABSTRACT

After the engineers built the computer networks, users had to build the social networks that made them useful. Listserv, the combined mailing list and file server, was an important tool for those interested in building network-based organizations. It first appeared on Bitnet, an academic network based on IBM computers. The early versions of Listserv became operational in the mid 1980s, and its early archives show how network users learned to use the software and, perhaps more importantly, how to manage network-based organizations.

Communication informelle (Goffman selon Grier)

A baisse les barrières :

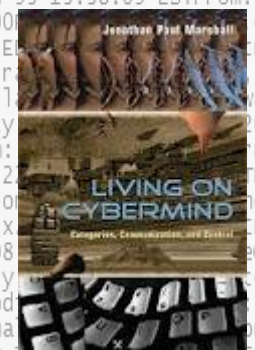
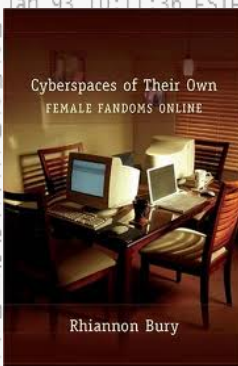
-Hiérarchiques

-Géographiques

-Disciplinaires

Mais pas totalement...(Marshall, Bury)

Influence du modérateur/administrateur



Rules

By posting to the list, you [agree](#) to adhere to the rules outlined in this document.

These rules, regarding what topics are [acceptable/unacceptable](#) and [commercial announcements](#) discussions. Do not reopen Pandora's box -- please.

Acceptable Topics

Topics which may appear on the list include:

- **software/hardware-related** issues
 - bugs: Reporting bugs in chemistry software and possible work-arounds
 - programs and utilities
 - availability: Information on the availability of particular software, data, etc.
 - hardware-related issues relevant to the computational chemistry community
- **announcements** of
 - new chemistry software
 - computational chemistry-related workshops and symposia
- **methods**
 - new methods and techniques in computational chemistry
 - Q&A: questions and answers about solving computational chemistry problems
- **opinions** about services and products

Commercial Announcements

Commercial software: software sold to anyone for use on the list, please respect the following rules:

- **Be brief** -- Short (25 lines or less) commercial posts
- **Be straightforward** -- The subject line should be clear
- **No reposting** -- Reposts of software announcements
- **No "vaporware"** -- Announcements of "vaporware" are not allowed.

Modérateur: Terms of service : privacy?, liste publique,

archives consultables.

Tensions académique/commercial

Re: Taxol: Fri, 1 Jan 93 14:11:05 ESTFrom: Francl Michel M <mfranl@cc.brynmawr.edu>Date: 4 Jan 93 12:33:36 -0800From: hcj@gull.munc.4 (Harry C. kfz-heidelberg.de>Subject: energy contribution of hbonds?Date: 06 Jan 1993 10:55:29 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: u
: CADD videosDate: Wed, 6 Jan 93 13:03:33 -0800From: chiremvl@andromeda!jeffb@uunet.UU.NET (Jeff Blaney)Subject: Re: Polygon-based solvent accessible surfacesDate: Thu, 7 Jan 93
!Date: 08 Jan 1993 09:19:39 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: replies to my posting about PDB searching methodsDate: F
vi@tiberius.tc.cornell.edu>From: scsupham@reading.ac.ukDate: Mon, 11 Jan 93 17:54:05 GMTSubject: DMol questionsDate: Mon, 11 Jan 1993 14:33 ESTFrom: WILLIAMS%XRAY2@ulkyvx02.loui
or doubled messagesDate: Wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@watson.ibm.comSubject: data-flow programs for molecular modelingDate: wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@
GAMESS and MOPACDate: Thu, 14 Jan 1993 10:42:35 -0500 (EST)From: HERMAN@
gov (Ron Shepard)Subject: Re: Cartesian vs Internal coordinatesDate: Fri, 15
0From: dmschn@bbbit.monsanto.comSubject: next Molecular Graphics Society Meet
n 93 15:29:22 +0100From: oosten@ruihml.LeidenUniv.nl (A.B. van Oosten)Subjec
O-STATE.EDU>Subject: RE: PC Survey RESULTSDate: Wed, 20 Jan 1993 15:47 CST
ke to test a program.Date: Thu, 21 Jan 93 12:19:42 +0100From: Inst.f. Phys.Ch
le RecurrenceDate: Fri, 22 Jan 1993 11:26:26 +0000From: BDIEAL <BDIEAL@camsc
Subject: This is a testDate: 26 Jan 1993 01:00:59 -0600 (CST)From: AHOLDER@VAX
a: 5; LROD/DD.ID=SSW.DWELROD/PRMD=U
3 20:38:08 GMTSubject: RE: XMD-Mac Converter...Date: Wed, 27 Jan 93 14:21:
93 14:47:36 -0500From: caves@tammy.harvard.eduDate: Thu, 28 Jan 1993 15:28:3
1993 14:23:55 +22305823 (EST)Date: Fri, 29 Jan 93 15:07:15 CSTFrom: shepard@
CHEM@OHSTVMA.ACS.OHIO-STATE.EDU>Subject: Re: Plotting Orbitals from a
radical cationDate: 1 Feb 1993 12:04:28 +0100From: cfat101
: youkha@biosym.comSubject: Summary: Internals & Non-BondsDate: Tue, 2 Feb
un.nl>Subject: Electronic Periodic TablesDate: 02 Feb 1993 14:36:03 -0500 (E
and NanotechnologiesDate: Wed, 3 Feb 93 10:46:20 MSTFrom: QINGSONG@minmet.la
OF TOLEDO" <DSMITH@uoft02.utoledo.edu>Subject: Re: Plotting Orbitals from a
3 +0100 (NFT)Date: 05 Feb 93 09:28:33 ESTFrom: Elliot King <71127.1231@compu
<bobby_clark@quickmail.clemson.edu>Subject: E-mail searchDate: 6 Feb 1993 10
500 (EST)From: spollack@ester.mse.uc.EDU (S.K. Pollack)Subject: Phosphazene
Date: Tue, 09 Feb 1993 21:39:58 -0500 (EST)From: "DR. DOUGLAS A. SMITH, UNIVERSITY OF TOLEDO" <DSMITH@uoft02.utoledo.edu>Subject: parallel workstations and serversDate: wed, 10
S.From: Zhou Feng <feng@lisboa.ks.uiuc.edu>Date: wed, 10 Feb 93 16:23:41 -0600Subject: parallel CHARMM?Date: wed, 10 Feb 93 15:46:43 -0800From: rickl@biosym.comSubject: DIBUG ad
T-2Subject: Re: ZINDO programDate: 11 Feb 1993 13:06:18 +0100From: schettler@chemix.mpi-stuttgart.mpg.deSubject: Mac summeryFrom: theresa@si.fi.ameslab.gov (Theresa Windus)S
/14031@hkuxa.hku.hk@OHSTVMA.ACS.OHIO-STATE.EDUSubject: MO Plotting program!Date: Fri, 12 Feb 93 09:48:41 CETFrom: Norbert Mueller <K360171%EDVZ.UNI-Linz.AC.%@OHSTVMA.ACS
: Re: X Windows for PC ..Date: Sat, 13 Feb 93 12:21:47 +0900From: Katushi Kobayashi <ikob@les.pc.uec.ac.jp>Date: Sat, 13 Feb 1993 14:47:09 +0100 (WET)From: PREINERT@biolan.u
ell.edu>Subject: MPW Fortran?Date: Tue, 16 Feb 93 13:28:40 ESTFrom: Kenneth McGreevy <kgreevy@hpldas1.sid.hp.com>Subject: Re: X windows for PC ..Date: Tue, 16 Feb 93 11:29:01 PS
TFrom: "w. Todd wipke" <wipke@SECS.UCSC.EDU>Subject: Final Call Summer Undergraduate Research Fellowship (SURF)Date: wed, 17 Feb 1993 14:15:16 -0500 (EST)From: "DR. DOUGLAS A. S
hu, 18 Feb 93 14:22:08 PSTFrom: raw@autodesk.com (Robert A Whiteside)Subject: Re: Question about PDB formatDate: Thu, 18 Feb 93 17:02:32 PSTFrom: fisher@scripps.edu (Cindy Fishe
feld chargesDate: Fri, 19 Feb 93 14:49:00 ESTFrom: "Janet DeI Bene" <FR042008@YSUB.YSU.EDU>Subject: BSSE calculationDate: Fri, 19 Feb 93 11:53:05 -0500From: G. Ravishanker <ravi
k.kjemi" <bjerkosa@kiami.unit.no>Subject: Summary: scaled freq for 5 and updat: Sun, 21 Feb 1993 20:51:10 +0100 (MET)Subject: Long Time-scale DynamicsDate: Mon, 22 Feb 93 16:49:
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ulz)subject: Stephen R. WilsonDate: Thu, 1 Apr 1993 16:33:29 +0200From: oles@gollum.uio.noSubject: BiosymDate: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNDRIT@memstvx1.memst.edus

USENET News Group ... NO!

- From: "R.G.A. Bone" <[rgab\(\)at\(\)purisima.molres.org](mailto:rgab()at()purisima.molres.org)>
- Subject: USENET News Group ... NO!
- Date: Wed, 27 Apr 94 11:24:39 -0700

Why not start CCL as a USENET NewsGroup ... ?
... because, even in 1994, there are still some of us who cannot access "USENET" (or, WWW, etc.) and for whom, therefore, a listserver like CCL is the only lifeline.
Many people in companies are behind so-called "firewalls" in which full internet-access (except e-mail) is denied.

Mutual shaping of users and technologies in a virtual community (Boczkowski)

RE:Nobel Prizers

- From: (Andrew Fant) <[fant\(+at+\)umbc3.umbc.edu](mailto:fant(+at+)umbc3.umbc.edu)> (+ at +) umbc3.umbc.edu
- Subject: RE:Nobel Prizers
- Date: Thu, 26 Sep 91 12:36:46 EDT

How about a joint Nobel to John Pople and Michael Dewar for their success in making computational tools available to the experimentalist and for their efforts to bring theoretical methods to bear on problems that non-physical chemists are interested (i.e. organic mechanisms).
I would not, however, want to be in the same room as the two of them as they wait to receive the award, or before they give their lectures.
Just another uninvolved opinion

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Date: 23 Feb 93 15:38:36-2300From: "Alexandre MICU P16A" <alex@ba
)-STATE.EDU>Subject: X-window terminal emulator for MacDate: Thu,
edu (Feng Chen)Subject: X-windows Server on MS-windowsDate: Thu, 2
12:08:57 +0100From: ole.swang@kjemi.uio.noSubject: language questi
: Sun, 28 Feb 93 13:44:41 GMT-2:00Date: Mon, 1 Mar 1993 15:25:19
)_B@LILLY.COM>Subject: new book on computational chemistryDate: Tue
mres.tn.cornell.edu>Subject: Re:Cache on the MacDate: Tue, 2 Mar 9
ject: PDB subdir organization?From: Jan Labanowski <jkl@ccl.net>Dat
atomic separationsFrom: sender@chemdcl.tau.ac.il (Senderowitz Hanoc
om: gallion@auriga.rose.brandeis.edu (steve gallion)Subject: Grow
ftware for PCDate: Fri, 12 Mar 93 04:51:15 GMTFrom: jim@quanta.phy.
: Sun, 14 Mar 93 11:06:13 +0100From: doelz@comp.bioz.unibas.ch (Re
;US@chemv2.mps.ohio-state.eduSubject: Problem with vibrational freq
stemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UN
: "STEPHEN R. HELLER" <srheller@asrn.arsusda.gov>Subject: Software
MA.ACS.OHIO-STATE.EDUSubject: First Congress of the ISTD (pa
: Program called GRIDDate: Fri, 19 Mar 93 14:33:18 ESTFrom: Ge
-0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Semic
armstadt.de (Hagen Dufner)Subject: efg in g92From: "Christopher J
: Gene A. Nelson)Subject: Batching files in MOPACFrom: zrfl0128@aw
Fe-0 calculationDate: Mon, 29 Mar 93 15:49:03 BSTFrom: rafapa@obel
Schulz)Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 -

full disclosure of methods?

- From: "DR. DOUGLAS A. SMITH, UNIVERSITY OF TOLEDO" <[DSMITH -AatT- uoft02.utoledo.edu](mailto:DSMITH-AatT-uoft02.utoledo.edu)>
- Subject: full disclosure of methods?
- Date: Sat, 26 Jun 1993 11:21:56 -0500 (EST)

Mark Thon discusses the issue of full disclosure of methods, mentioning that it brings in basic techniques and is followed by those who use it for the difference.

Re: full disclosure of methods?

- From: [st-amant { *at * } cgl.ucsf.edu](mailto:st-amant{*at*}@cgl.ucsf.edu) (Alain St-Amant)
- Subject: Re: full disclosure of methods?
- Date: Sat, 26 Jun 93 12:21:56 -0700

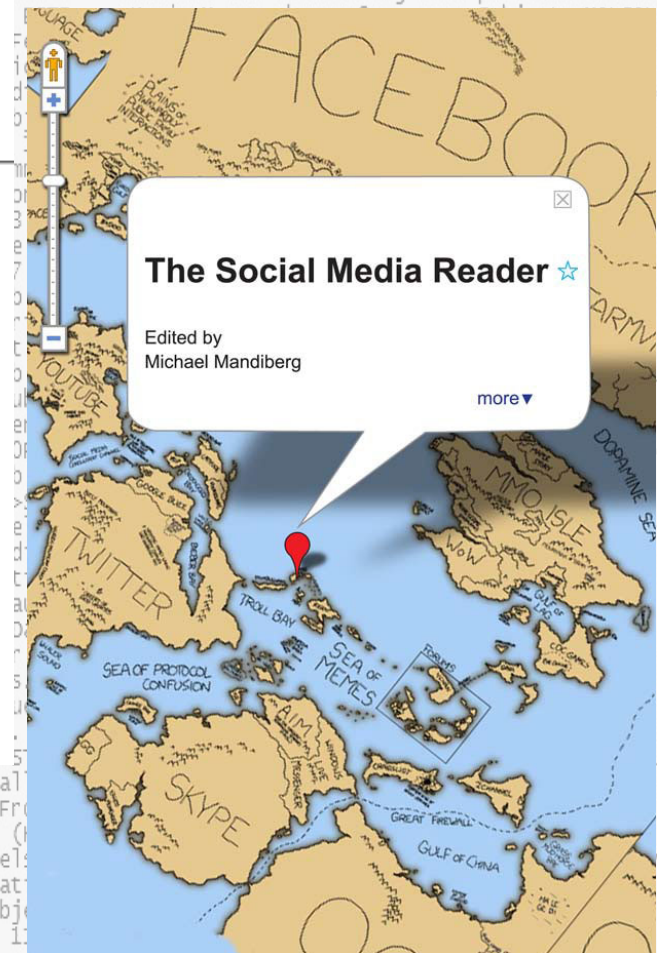
Douglas Smith recently wrote in the current discussion on the disclosure of parameters: > Besides, who ever said we had to reveal all our secrets and make them > readily available and accessible? When software copyrights and patents > really provide adequate protection, maybe I will agree with that attitude. I'll assume that Dr. Smith is referring to the specific algorithms that are implemented that make the program more efficient but do not affect the final results. In which case, I might agree. Of course, I couldn't disagree more if he is referring to some development in the methodology that actually affects the final results in any way. The point that interests me however, is the question of software copyrights and patents to which Dr. Smith alludes. I have been trying to get a feel for what can be copyrighted and patented and I get a different answer from everyone. Can only specific code be copyrighted or can the structure and algorithms be copyrighted as well? How 'modified' should code be before it can be called legally (and ethically if anyone is interested in expressing an opinion) a new program? Or is it simply forbidden for code to "evolve" into a new program? I will summarize to the net any e-mail sent to me, but I think that this would make for an interesting discussion and it would be as interesting to hear how

- From: [st-amant { *at * } cgl.ucsf.edu](mailto:st-amant{*at*}@cgl.ucsf.edu) (Alain St-Amant)
- Subject: Re: full disclosure of methods?
- Date: Sat, 26 Jun 93 12:21:56 -0700

Douglas Smith recently wrote in the current discussion on the disclosure of parameters: > Besides, who ever said we had to reveal all our secrets and make them > readily available and accessible? When software copyrights and patents > really provide adequate protection, maybe I will agree with that attitude. I'll assume that Dr. Smith is referring to the specific algorithms that are implemented that make the program more efficient but do not affect the final results. In which case, I might agree. Of course, I couldn't disagree more if he is referring to some development in the methodology that actually affects the final results in any way. The point that interests me however, is the question of software copyrights and patents to which Dr. Smith alludes. I have been trying to get a feel for what can be copyrighted and patented and I get a different answer from everyone. Can only specific code be copyrighted or can the structure and algorithms be copyrighted as well? How 'modified' should code be before it can be called legally (and ethically if anyone is interested in expressing an opinion) a new program? Or is it simply forbidden for code to "evolve" into a new program? I will summarize to the net any e-mail sent to me, but I think that this would make for an interesting discussion and it would be as interesting to hear how

Hacker and Troller as Trickster (Coleman)

-Religious wars: Flaming, Trolling



Subject: energy contribution of hbonds?Date: 06 Jan 1993 10:55:29 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: u
CADD videosDate: wed, 6 Jan 93 13:03:33 -0800From: chiremv@andromeda.jeffb@uunet.UU.NET (Jeff Blaney)Subject: Re: Polygon-based solvent accessible surfacesDate: Thu, 7 Jan 93
!Date: 08 Jan 1993 09:19:39 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: replies to my posting about PDB searching methodsDate: F
vi@tiberius.tc.cornell.edu>From: scsupham@reading.ac.ukDate: Mon, 11 Jan 93 17:54:05 GMTSubject: DMOI questionsDate: Mon, 11 Jan 1993 14:33 ESTFrom: WILLIAMS%XRAY2@ulkyvxo2.loui
or doubled messagesDate: wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@watson.ibm.comSubject: data-flow programs for molecular modelingDate: wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@
GAMES and MOPACDate: Thu, 14 Jan 1993 10:42:35 -0500 (EST)From: HERMAN@ULNA.BWH.HARVARD.EDUSubject: RE:HELPPDate: Thu, 14 Jan 1993 11:18:26 -0500From: jle@world.std.com (Joe
ov (Ron Shepard)Subject: Re: Cartesian vs Internal coordinatesDate: Fri, 15 Jan 93 06:48 CDTFrom: CUNARIT%MEMSTVX1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDUSubject: Steric strain at T
OFrom: dmschn@bbt.monsanto.comSubject: next Molecular Graphics Society MeetingFrom: m.e. <harboww@chemres.tn.cornell.edu>Subject: UHF calc's on diradicals/TSDDate: Mon. 18 Jan 9
n 93 15:29:37 -0500 (EST)From: "D. Mathieu" <DEWINDT%FRSAC11.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>Subject: Re: plot
O-STATE.EDU>Subject: RE: FC Survey RESULTSDate: Wed, 20 Jan 1993 12:47 CSTFrom: "JORGE
ke to test a program.Date: Thu, 21 Jan 93 12:19:42 +0100From: Inst.f.Phys.Chem. I <pci@pi
Jan 93 13:27:12 GMTFrom: "D. Mathieu" <DEWINDT%FRSAC11.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>
le RecurrenceDate: Fri, 13 Jan 1993 13:58:13 ESTFrom: "BDIEAL@camsci.com" <BDIEAL@camsci.com>Subject
From: arne@mango.met.kl.se (Arne Etofsson)Subject: Re: charmm and SGIs - charmm newsgroup
Subject: This is testDate: 26 Jan 1993 07:20:59 -0600 (CST)From: AHOLDER@VAX1.UMKC.EDUSul
ate: 27 Jan 93 05:59:32 -0700From: /PN=DAVID.W.ELROD/DD,SD=SSW.DWELROD/PRND=UPJOHN/ADMD=TI
3 20:38:47 ESTFrom: RE: Arne EtofssonDate: Thu, 28 Jan 1993 14:21:29 -0700From: <
93 14:47:36 -0500From: caves@tammy.harvard.eduDate: Thu, 28 Jan 1993 15:28:31 PSTFrom: V
1993 14:23:55 +22305823 (EST)Date: Fri, 29 Jan 93 15:07:15 CSTFrom: shepard@dirac.tcg.an
CHEM.CMU.EDU>Subject: Gaussian and excited statesDate: Fri, 29 Jan 93 16:35:12 ESTFrom
radomski@cam.ac.ukSubject: Summary: Internals & Non-BondsDate: Tue, 2 Feb 93 11:12:51 <
un.nl>Subject: Electronic Periodic TablesDate: 02 Feb 1993 14:36:03 -0500 (EST)From: ZUR
and NanotechnologiesDate: wed, 3 Feb 93 10:46:20 MSTFrom: QINGSONG@minmet.1
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3 +0100 (NFT)Date: 05 Feb 93 09:28:33 ESTFrom: Elliot King <71127.1231@comp
<bobby_clark@quickmail.clemson.edu>Subject: E-mail searchDate: 6 Feb 1993 1
500 (EST)From: "D. Mathieu" <DEWINDT%FRSAC11.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>
Date: Tue, 09 Feb 1993 21:39:59 -0500 (ST)From: DR. DOUGLAS A. SMITH, UNI
S.From: Zhou Feng <feng@lisboa.ks.uiuc.edu>Date: wed, 10 Feb 93 16:23:41 -0
T-2Subject: Re: ZINDO programDate: 11 Feb 1993 13:06:18 +0100From: sch
714031%h@uiowa.eduSubject: MO Plotting program!
t: Re: X Windows for PC ..Date: sat, 13 Feb 93 12:21:47 +0900From: Katushi
ell.edu>Subject: MPW Fortran?Date: Tue, 16 Feb 93 13:28:40 ESTFrom: Kenneth
TFFrom: "w. Todd Winkler" <WINKER@SEC@UCSC.EDU>Subject: Final Call Summer Unde
hu, 18 Feb 1993 10:09:36 ESTFrom: Robert A Whiteside)Subje
feld chargesDate: Fri, 19 Feb 93 14:49:00 ESTFrom: "Janet Del Bene" <FR0420
k Kjemi" <bjerkese@kjemi.unit.no>Subject: Summary: Scanned freq for S and HD
: Carl J. Jorgensen <carlj@chem.nyu.edu>Date: Thu, 18 Feb 93 17:21 EDTFrom: <PODO
(g)Subject: Re: X Window Terminal Emulator for MacDate: Thu, 25 Feb 93 17:19
nl.govSubject: X-window terminal emulator for MacDate: Thu, 25 Feb 93 17:19
d.harvard.edu (jill cheney)Subject: Computer Program to Evaluate Wigner 3j
semiempirical integrals for Gaussian basis functionsDate: Thu, 25 Feb 93 17:19
n.desubject: Expert Know-how wanted !Date: 02 Mar 1993 08:13:18 -0500 (EST
ate.Edu (Gene Carter)Subject: Co MD parameters.Date: Tue, 2 Mar 93 17:22:5
lling Software: Does anyone have STELLA?Date: 04 Mar 1993 17:08:31 -0500 (E
ar 93 17:08:31 -0500 (EST)From: <SML108@PSUVM.PSU.E
secc.fi.cnr.it>Subject: MO Theory Made VisibleDate: Tue Mar 09 11:23:12 1993
uplingDate: Thu, 11 Mar 93 18:54 EDTFrom: <PODOSNNA%NYUACF1.BITNET@OHST
r 1993 02:33:00 -0800 (PST)From: Thomas Schwan <tom@cas.washington
MA.ACS.OHIO-STATE.EDU>Subject: Re: Cartesian vs Internal coordinates in G92Date
, 15 Mar 1993 21:55:05 -0600 (CST)From: Chris Parkinson <mbdtscp@hpc.ch.man
ar 1993 13:58:36 -0400From: ZSHI@ac.dal.caSubject: Information about IBM RS
st Giron <stgiron@chem.tn.cornell.edu>Date: Thu, 18 Mar 93 10:40
:11 -0500 (EST)From: "D. Mathieu" <DEWINDT%FRSAC11.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>
23 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Announcing
.ml>Subject: What about simulated annealing?Date: wed, 24 Mar 93 14:11:32 +
ject: SC&A Conference speakers - thanksDate: Thu, 25 Mar 93 10:18:48 -0500From: au195@cleveland.freenet.edu (Dr. Gene A. Nelson)Subject: Batching files in MOPACFrom: zrfl0128@aw
MO@CHEMNA.DICHI.UNINA.ITSubject: looking for ACES programFrom: Robert Laird <mbdtssl@hpb.ch.man.ac.uk>Subject: Fe-O calculationDate: Mon, 29 Mar 93 15:49:03 BSTFrom: rafapa@obel
uk>Subject: Polyrate queryDate: Tue, 30 Mar 1993 19:31:32 +0200From: c62@aixfile1.urz.uni-heidelberg.de (Andreas Schulz)Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 -
ulz)Subject: Stephen R. WilsonDate: Thu, 1 Apr 1993 16:33:29 +0200From: oles@gollum.uio.noSubject: BiosymDate: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNARIT@memstvx1.memst.edu

- Controverse scientifique

: utile pour l'historien,

oblige les acteurs à se

dévoiler.

- Sociologie pragmatique

des épreuves : la

situation de crise

(tensions) permet

d'observer des

changements de

structure...et rend les

acteurs bavards.

full disclosure of methods?

- From: "DR. DOUGLAS A. SMITH, UNIVERSITY OF TOLEDO" <[DSMITH -AatT- uoft02.utoledo.edu](mailto:DSMITH-AatT-uoft02.utoledo.edu)>
- Subject: full disclosure of methods?
- Date: Sat, 26 Jun 1993 11:21:56 -0500 (EST)

Mark Thompson recently wrote, regarding the SAM1 topic currently under discussion:
>Let me address the more fundamental issue that this topic
>brings forth. I share Graham Hurst's concerns. One of the

Re: full disclosure of methods?

- From: [st-amant { *at * } cgl.ucsf.edu](mailto:st-amant{*at*}cgl.ucsf.edu) (Alain St-Amant)
- Subject: Re: full disclosure of methods?
- Date: Sat, 26 Jun 93 12:21:56 -0700

Douglas Smith recently wrote in the current discussion on the disclosure of parameters:
> Besides, who ever said we had to reveal all our secrets and make them
> readily available and accessible? When software copyrights and patents
> really provide adequate protection, maybe I will agree with that attitude.
I'll assume that Dr. Smith is referring to the specific algorithms that are implemented that make the program more efficient but do not affect the final results. In which case, I might agree.
Of course, I couldn't disagree more if he is referring to some development in the methodology that actually affects the final results in any way.
The point that interests me however, is the question of software copyrights and patents to which Dr. Smith alludes. I have been trying to get a feel for what can be copyrighted and patented and I get a different answer from everyone. Can only specific code be copyrighted or can the structure and algorithms be copyrighted as well? How 'modified' should code be before it can be called legally (and ethically if anyone is interested in expressing an opinion) a new program? Or is it simply forbidden for code to "evolve" into a new program?
I will summarize to the net any e-mail sent to me, but I think that this would make for an interesting discussion and it would be as interesting to hear how

Is the CCL a public sphere ?

-Disregard of status

-Domain of common concern

-Inclusivity

-Independence from power

-Influence political action through

discussion

(Kelty)

The Structural Transformation of the Public Sphere

An Inquiry into a Category of Bourgeois Society

Jürgen Habermas

translated by Thomas Burger
with the assistance
of Frederick Lawrence



THE CULTURAL SIGNIFICANCE OF FREE SOFTWARE

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