Managing open scientific collaboration nmrlipids.blogspot.fi

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What have we done: **Open collaboration platfrom to resolve lipid structures**

Why: Communication possibilities through the Internet allow more effective information sharing than traditional scientific publication system
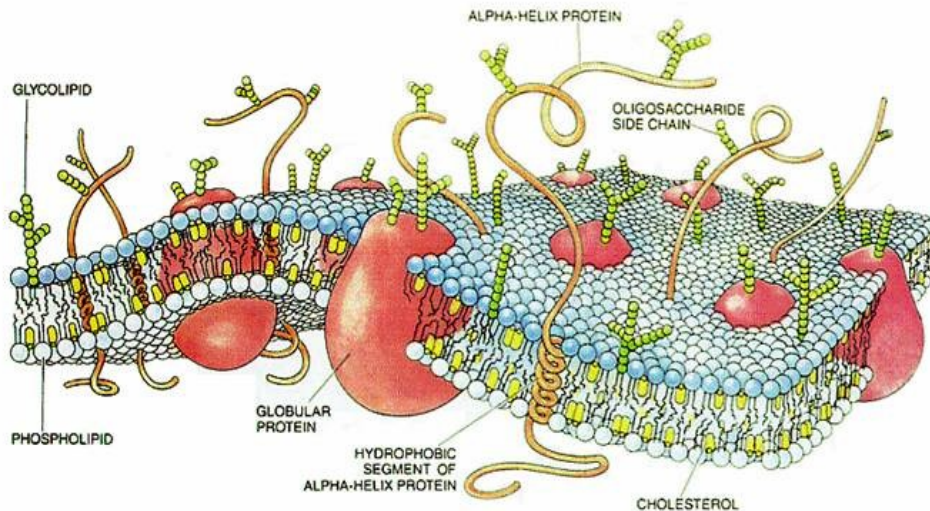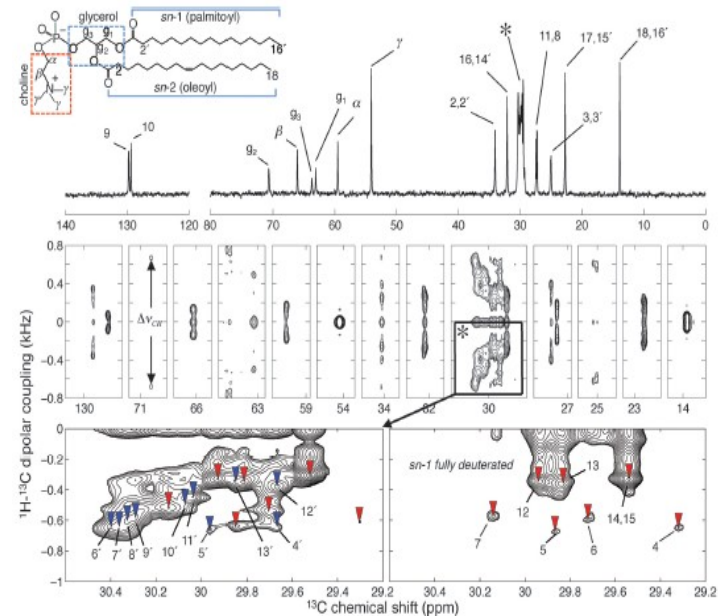
How did it work?:
Pretty well.

GENERAL GOAL IN THE FIELD: ATOMISTIC RESOLUTION STRUCTURE OF CELL MEMBRANE

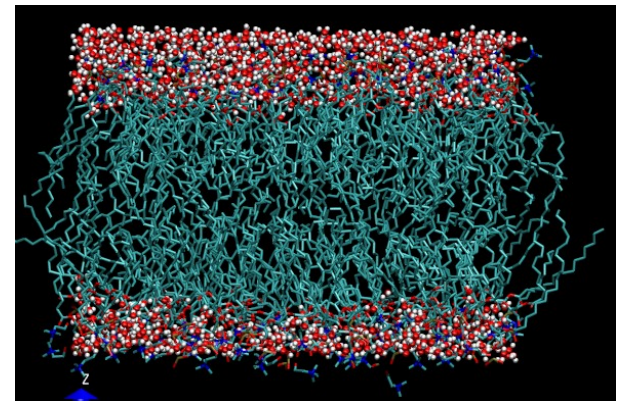Lipid vesicles as a simple model for a cell membrane:

How cholesterol affects cell membranes?
Do ions partition into cell membrane?

Nuclear Magnetic Resonance (NMR) experiment:

Molecular dynamics simulation:

# Why to do MD simulation of lipid bilayers?

(one motivation)

NMR (order) parameters related to the structure are experimentally known with high accuracy
Scientific question: What is the atomistic resolution structure of the molecule?

Traditional approach: Use intuition and relatively complicated mathematical models to construct structures which would reproduce the measured parameters

MD simulation approach: MD model which reproduces the measured parameters gives automatically a realistic structure

Sampled single molecule structures in lipid bilayer
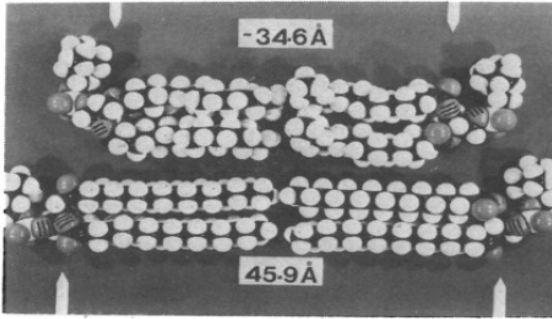
Seelig and Seelig Biochemistry 23 (1974) 4639
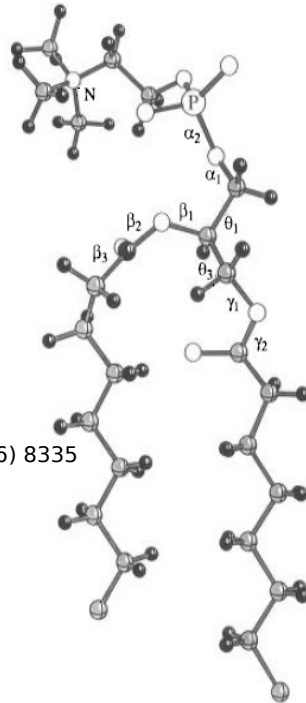
Hong et al.
Biochemistry 35 (1996) 8335

20% DMTAP   Neutral   50% DMPG
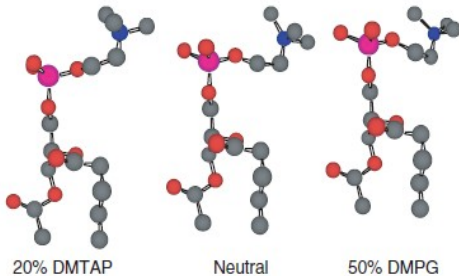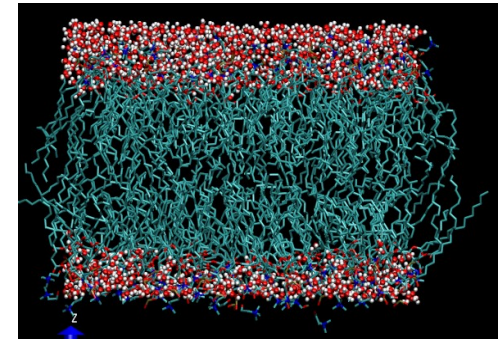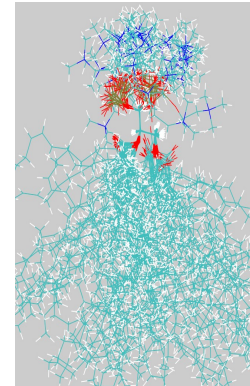
Semchyschyn and Macdonald Magn. Res. Chem. 42 (2004) 89

Advantages:
More feasible, 3D structure for visualization, the model can be used to answer also other questions like interaction with other molecules and energetics

Important note:
The model has to correspond experimental reality

ORIGINAL OBSERVATIONS
(simplified presentation to describe the situation)
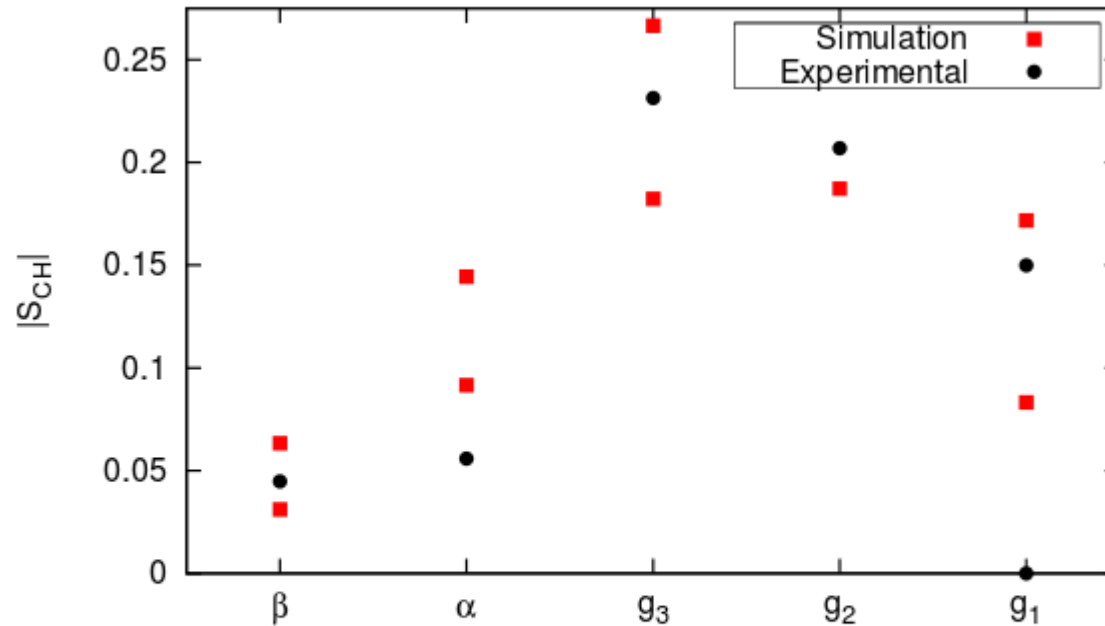
FIG. 2: Order parameteres from simulations and experiments for glycerol and choline groups of POPC. Experimental values taken from [7].

Lipid structures are not correct.
How about the other available lipid models?
How to fix this?

OPTIONS IN TRADITIONAL SCIENTIFIC DISCOURSE

Publish results and hope that the field reacts
+ Doable
 - Only negative result, not real progress
 - Field reacts very slow (if at all) to unexpected and unconvenient results

Test all the models and/or improve the existing
 - Too much work even for a small research group

OPEN COLLABORATION APPROACH PLANNED WITH MARKUS MIETTINEN

Manuscript describing the observations was written and published in ArXiv

O.H.S. Ollila, Response of the hydrophilic part of lipid membranes to changing conditions - a critical comparison of simulations to experiments
http://arxiv.org/abs/1309.2131

Open collaboration to improve and progress the manuscript was started at:
http://nmrlipids.blogspot.fi/

- The project is progressed and discussed as an open collaboration only through the blog
- A regular journal articles are written when appropriate
- People who have contributed through the blog format will be author's

Matching lipid force fields with NMR data

Collaboration platform to find a lipid force field that matches the measured NMR order parameters.

Home	Authors	To Do List	Data contributions	Downloads	Publications	

Monday, March 9, 2015

Current status of the project

9.3.2015 Current and future activity **post was published.**

6.3.2015 Samuli will talk about this project in the event organized by the Open Knowledge Finland (OKFFI) on 10.3.2015 in University of Helsinki. **There will also live stream from the event through this link** http://vn-rec.it.helsinki.fi

6.2.2015 The first draft of the ion-lipid interaction manuscript was published.

16.1.2015 Towards first submission to journal **post was published.**

16.1.2015 The current version of the new manuscript is now updated to arXiv http://arxiv.org/abs/1309.2131v2. **There will be soon a new post about the further proceeding.**

23.12.2014 New version of the manuscript (2) **post was published.**

21.11.2014 New manuscript written on the results reported in this blog is available for commenting: New version of the manuscript. **The manuscript covers only the results for fully hydrated bilayers, effect of dehydration and effect of cholesterol. A separate manuscript will be written about ion-lipid**

Latest comments

- ad 1) You are right that the position of the peak … - **Peter Heftberger**
- I have now updated more experimental datapoints in… - **Samuli Ollila**
- 1. After reading the publications more carefully I… - **Samuli Ollila**
- Hi, Here are the averaged data using every frame … - **fernando favela**
- Hi, To re-open the discusion about the publicatio… - **Hubert Santuz**

Chronological list of all posts

20. Current and future activity
19. The first draft of the ion-lipid interaction manuscript
18. Towards first submission to journal
17. New version of the manuscript (2)
16. New version of the manuscript
15. About glycerol conformations

What have we done: Open collaboration platfrom to resolve lipid structures

Why: Communication possibilities through the Internet allow more effective information sharing than traditional scientific publication system

How did it work?:
Pretty well.

WHY DID WE DO IT?

- Fundamental idea behind scientific publishing is to spread and advance knowledge as effectively as possible.
- Internet is better for this purpose than printed articles
- Scanning articles to the internet is not the optimal solution

Some advantages of our approach

- Self-correcting is more efficient
- Otherwise unpublished small pieces of information can be utilized as a part of larger entity
- The whole process of study is openly documented and can be studied later

WHY DID WE DO IT?

- Positive examples:

Polymath Project

From Wikipedia, the free encyclopedia

The **Polymath Project** is a collaboration among mathematicians to solve important and difficult mathematical problems by coordinating many mathematicians to communicate with each other on finding the best route to the solution. The project began in January 2009 on Tim Gowers' blog when he posted a problem and asked his readers to post partial ideas and partial progress toward a solution. This experiment resulted in a new answer to a difficult problem, and since then the Polymath Project has grown to describe a particular process of using an online collaboration to solve any math problem.

Gowers's Weblog
Mathematics related discussions

« A Tricki issue   Background to a Polymath project »

Is massively collaborative mathematics possible?

Of course, one might say, there are certain kinds of problems that lend themselves to huge collaborations. One has only to think of the proof of the classification of finite simple groups, or of a rather different kind of example such as a search for a new largest prime carried out during the downtime of thousands of PCs around the world. But my question is a different one. What about the solving of a problem that does not naturally split up into a vast number of subtasks? Are such problems best tackled by n people for some n that belongs to the set $\{1, 2, 3\}$? (Examples of famous papers with four authors do not count as an interesting answer to this question.)

It seems to me that, at least in theory, a different model could work: different, that is, from the usual model of people working in isolation or collaborating with one or two others. Suppose one had a forum (in the non-technical sense, but quite possibly in the technical sense as well) for the online discussion of a particular problem. The idea would be that anybody who had anything whatsoever to say about the problem could chip in. And the ethos of the forum — in whatever form it took — would be that comments would mostly be kept short. In other words, what you would *not* tend to do, at least if you wanted to keep within the spirit of things, is spend a month thinking hard about the problem and then come back and write ten pages about it. Rather, you would contribute ideas even if they were undeveloped and/or likely to be wrong.

This suggestion raises several questions immediately. First of all, what would be the advantage of proceeding in this way? My answer is that I don't know for sure that there *would* be an advantage. However, I can see the following potential advantages.

(i) Sometimes luck is needed to have the idea that solves a problem. If lots of people think about a problem, then just on probabilistic grounds there is more chance that one of them will have that bit of luck.

(ii) Furthermore, we don't have to confine ourselves to a purely probabilistic argument: different people know different things, so the

Linux

```
From: torv...@klaava.Helsinki.FI (Linus Benedict Torvalds)
Newsgroups: comp.os.minix
Subject: What would you like to see most in minix?
Summary: small poll for my new operating system
Keywords: 386, preferences
Message-ID: <1991Aug25.205708.9541@klaava.Helsinki.FI>
Date: 25 Aug 91 20:57:08 GMT
Organization: University of Helsinki
Lines: 20


Hello everybody out there using minix -

I'm doing a (free) operating system (just a hobby, won't be big and
professional like gnu) for 386(486) AT clones.  This has been brewing
since april, and is starting to get ready.  I'd like any feedback on
things people like/dislike in minix, as my OS resembles it somewhat
(same physical layout of the file-system (due to practical reasons)
among other things).

I've currently ported bash(1.08) and gcc(1.40), and things seem to work.
This implies that I'll get something practical within a few months, and
I'd like to know what features most people would want.  Any suggestions
are welcome, but I won't promise I'll implement them :-)

                Linus (torv...@kruuna.helsinki.fi)

PS.  Yes - it's free of any minix code, and it has a multi-threaded fs.
It is NOT protable (uses 386 task switching etc), and it probably never
will support anything other than AT-harddisks, as that's all I have :-(.
```

What have we done: Open collaboration platform to resolve lipid structures

Why: Communication possibilities through the Internet allow more effective information sharing than traditional scientific publication system

How did it work?:
Pretty well.

Speculative problems related to the Open Collaboration approach:

- No existing platforms, culture and tools for this kind of approach
- No one participates
- Spamming and trolling
- Too many useless (messy, unclear, or off-topic) contributions suffocate the project
- Major personal conflicts lead to internet fight
- Authors without significant scientific contribution in final publication
- Influental people get angry and try to sabotage our careers
- Someone steals the ideas and publishes them as own

NONE OF THESE ISSUES HAS BEEN A REAL PROBLEM!

HOW DID WE DEAL WITH THE EXPECTED PROBLEMS:

- No existing platforms, culture and tools for this kind of approach

Which kind of platform we need?
I do not know.
What are the best tools?
I do not know.
What are the best practises and rules?
I do not know.

CONCLUSION: We just have to do it somehow to gather practical experience.
Our philosophy: we do everything with minimun effort and see if it works

Blog format was chosen due to the success of Polymath.
Other tools used: Dropbox, GitHub, Figshare, Zenodo

HOW DID WE DEAL WITH THE EXPECTED PROBLEMS:

- No one participates

Funding is currently based on peer-reviewed publications → we need to make peer-reviewed publications to get people involved.

Who will be authors and in which order → The authorship is offered everyone who comment the blog. The acceptance is based on the self assesment on the scientific contribution. The order is alphaphetical.

The project was advertized with email invitations and in conference presentations. Also some people noticed the original arXiv publication.

HOW DID WE DEAL WITH THE EXPECTED PROBLEMS:

Tuesday, September 10, 2013

The manuscript is now available. What next?

This blog has been started to make improvements on the manuscript titled "Response of the hydrophilic part of lipid membranes to changing conditions — a critical comparison of simulations to experiments", written by O. H. Samuli Ollila, and openly available at http://arxiv.org/abs/1309.2131.

Alexander Lyubartsev September 13, 2013 at 2:01 PM

This is interesting idea to test a new way of publishing.

My first question, after looking on the figures, what is uncertainty of the experimental (and also simulation) results? Can we be sure that they are, for example, within 0.02 for the order parameters?

Another question is sign of the order parameters. In some cases experimental order parameters for lipid headgroups are reported with sing (I have in hand references for DMPC, JACS 119, 796 (1997) and Langmuir 19, 10468 (2003), may be there exist such data for POPC), this would be even a stronger test on suitability of a force field.

Matti Javanainen September 13, 2013 at 3:53 PM

Here are the results I calculated for three bilayer systems with the Slipids force field:

1) Pure POPC, 512 lipids, 298K, 40 waters/lipid, 150mM NaCl, PME, 300ns, Slipids
2) POPC+10%Chol, 288 PCs, 310K, 45 waters/lipid, 150mM NaCl, PME, 200ns, Slipids
3) DPPC+10%Chol, simulation parameters as above

The plot is available at https://dl.dropboxusercontent.com/u/6808285/hg_order.pdf

and here's the raw data:

- ~295 comments
- 23 participants

Editors:

O. H. Samuli Ollila
Markus S. Miettinen

Contributors:

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Olle Edholm
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Jukka Määttä
Vasily Oganesyan
Georg Pabst
O. H. Samuli Ollila
Marius Retegan
Tomasz Rog
Hubert Santuz
Peter Tieleman
Joona Tynkkynen
Alexander Vogel
Mark Wilson

HOW DID WE DEAL WITH THE EXPECTED PROBLEMS:

ALMOST READY:

Towards atomistic resolution structure of phosphatidylcholine glycerol backbone and choline headgroup at different ambient conditions

Alexandru Botan,[*] Fernando Favela, Patrick Fuchs,[†] Matti Javanainen,[‡] Waldemar Kulig,[‡] Antti Lamberg,[§] Markus S. Miettinen,[¶] Luca Monticelli,[||] Jukka Määttä,[**] O. H. Samuli Ollila,[††] Marius Retegan,[‡‡] Tomasz Rog,[‡] Hubert Santuz,[§§] and Joona Tynkkynen[‡]

FIRST DRAFT HAS BEEN WRITTEN:

Binding of cations to phospholipid bilayers

Andrea Catte,[*] Matti Javanainen,[†] Markus S. Miettinen,[‡] Vasily S. Oganesyan,[§] and O. H. Samuli Ollila[¶]

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Peter Tieleman
Joona Tynkkynen
Alexander Vogel
Mark Wilson

HOW DID WE DEAL WITH THE EXPECTED PROBLEMS:

These have not happened (yet):

- Spamming and trolling
- Too many useless (messy, unclear, or off-topic) contributions suffocate the project
- Major personal conflicts lead to internet fight
- Authors without significant scientific contribution in final publication
- Influental people get angry and try to sabotage our careers

This is not possible:

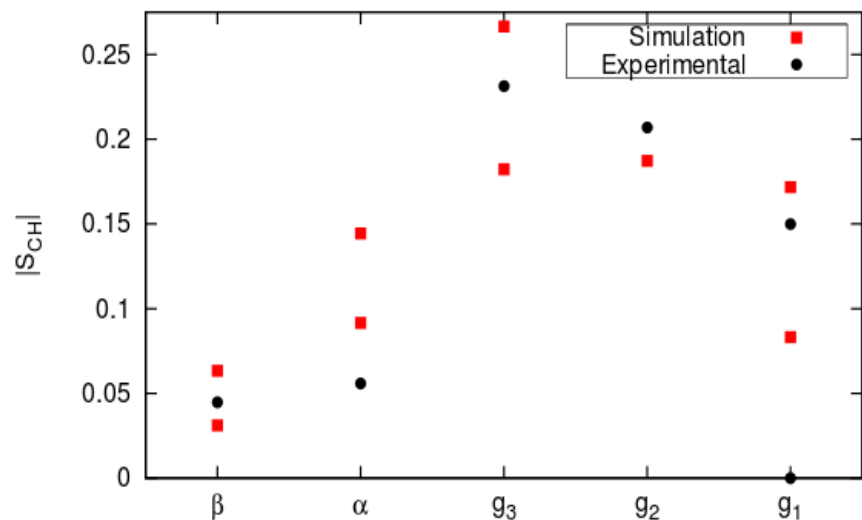- Someone steals the ideas and publishes as own

Because published work cannot be stolen.
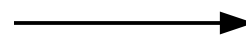
WAS IT USEFUL?

FIG. 2: Order parameteres from simulations and experiments for glycerol and choline groups of POPC. Experimental values taken from [7].

Open collaboration

ADDITIONAL THOUGHTS AND OPEN QUESTIONS

About tools:

Blog as a discussion forum
  - Works but not optimal
  - There would be room for application development here!

GitHub as a working directory
  - This seems very good
  - This will be probably used more in the future
  - Many people are not familiar with Git system yet.

Zenodo.org (repository ran by CERN)
  - Good for permanent storage
  - Free, no quota, 2GB file size limit, gives doi

Recent and promising initiative thewinnower.com
  - Gives doi:s for blogs

ADDITIONAL THOUGHTS AND OPEN QUESTIONS

About publishing in journal:

In principle traditional scientific Journals might not accept this kind of work since it is already published.

About getting people involved:

What are the main motivations to participate?
What are the main barriers to not participate?

There is very little criticism:

How to get more critical, peer review like comments?

Generation gap

This approach is more natural for younger generation

What is the most effective discussion culture?

1. **Be polite and constructive.** Polymath projects are team efforts, and any unnecessary conflict between participants is likely to impact that effort negatively. Criticism of a mathematical argument is welcomed, but personal criticisms should be avoided if possible.

Polymath
vs.
Linux

Date Sat, 13 Jul 2013 15:40:24 -0700
Subject Re: [GIT pull] x86 updates for 3.11
From Linus Torvalds <>

On Sat, Jul 13, 2013 at 4:21 AM, Thomas Gleixner <tglx@linutronix.de> wrote:
>
>   * Guarantee IDT page alignment

What the F*CK, guys?

This piece-of-shit commit is marked for stable, but you clearly never even test-compiled it, did you?

Because on x86-64 (the which is the only place where the patch matters), I don't see how you could have avoided this honking huge warning otherwise:

  arch/x86/kernel/traps.c:74:1: warning: braces around scalar initializer [enabled by default]
    gate_desc idt_table[NR_VECTORS] __page_aligned_data = { { { { 0, 0 } } }, };

  arch/x86/kernel/traps.c:74:1: warning: (near initialization for 'idt_table[0].offset_low') [enabled by default]
  arch/x86/kernel/traps.c:74:1: warning: braces around scalar initializer [enabled by default]
  arch/x86/kernel/traps.c:74:1: warning: (near initialization for 'idt_table[0].offset_low') [enabled by default]
  arch/x86/kernel/traps.c:74:1: warning: excess elements in scalar initializer [enabled by default]
  arch/x86/kernel/traps.c:74:1: warning: (near initialization for 'idt_table[0].offset_low') [enabled by default]
and I don't think this is compiler-specific, because that code is crap. The declaration for gate_desc is very very different for 32-bit and 64-bit x86 for whatever braindamaged reasons.

Seriously, WTF? I made the mistake of doing multiple merges back-to-back with the intention of not doing a full allmodconfig build in between them, and now I have to undo them all because this pull request was full of unbelievable shit.

And why the hell was this marked for stable even *IF* it hadn't been complete and utter tripe? It even has a comment in the commit message about how this probably doesn't matter. So it's doubly crap: it's *wrong*, and it didn't actually fix anything to begin with.

There aren't enough swear-words in the English language, so now I'll have to call you perkeleen vittupää just to express my disgust and frustration with this crap.

          Linus

CONCLUSIONS

Open collaboration approach has been successful at least in operation system development, mathematics and biophysical chemistry

Open collaboration approach will be successful in wide range of different fields

We should understand what is the main barrier to implement and participate to these projects

ACKNOWLEDGEMENTS

Open research approach

Markus Miettinen

The Emil Aaltonen Foundation

THANKS FOR YOUR ATTENTION!