The State of PsiForum

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November 9, 2018

PSI4

OPEN-SOURCE QUANTUM CHEMISTRY

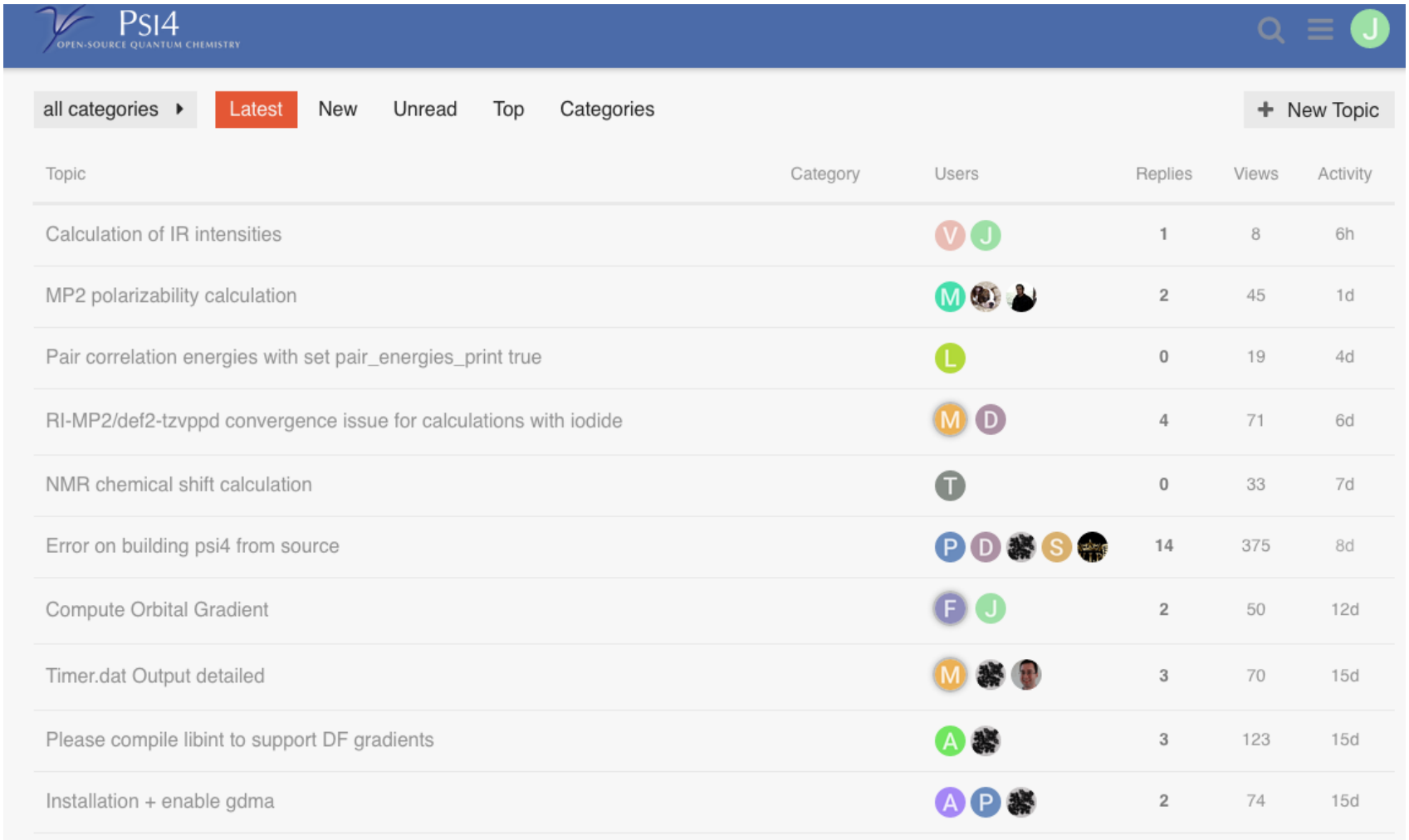
news | manual | developers | downloads

Psi4Education | contacts | history | user forum

PSI4 User Survey! (respond by 1 Nov)

PSI4NUMPY Paper!

Our latest paper shows how a combination of PSI4 and NUMPY can be used to facilitate the rapid development of clear, understandable code for electronic structure theory, and presents a set of reference implementations. Available from the *Journal of Chemical Theory and Computation*


Psi4
OPEN-SOURCE QUANTUM CHEMISTRY
J
all categories
Latest
New
Unread
Top
Categories
+ New Topic
Topic
Category
Users
Replies
Views
Activity
Calculation of IR intensities
1
8
6h
MP2 polarizability calculation
2
45
1d
Pair correlation energies with set pair_energies_print true
0
19
4d
RI-MP2/def2-tzvppd convergence issue for calculations with iodide
4
71
6d
NMR chemical shift calculation
0
33
7d
Error on building psi4 from source
14
375
8d
Compute Orbital Gradient
2
50
12d
Timer.dat Output detailed
3
70
15d
Please compile libint to support DF gradients
3
123
15d
Installation + enable gdma
2
74
15d

Procedure

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  - Questions about third-party programs, but not their Psi interfaces
  - Unintelligible questions
- Some threads have multiple questions, if the topic changes, e.g., user asks what the default SAPT(DFT) functional is, but asks about the sensitivity of SAPT(DFT) to choice of functional as a follow-up

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- Made rough logs of who posted where when
- Tons of data! What follows is highly distilled.

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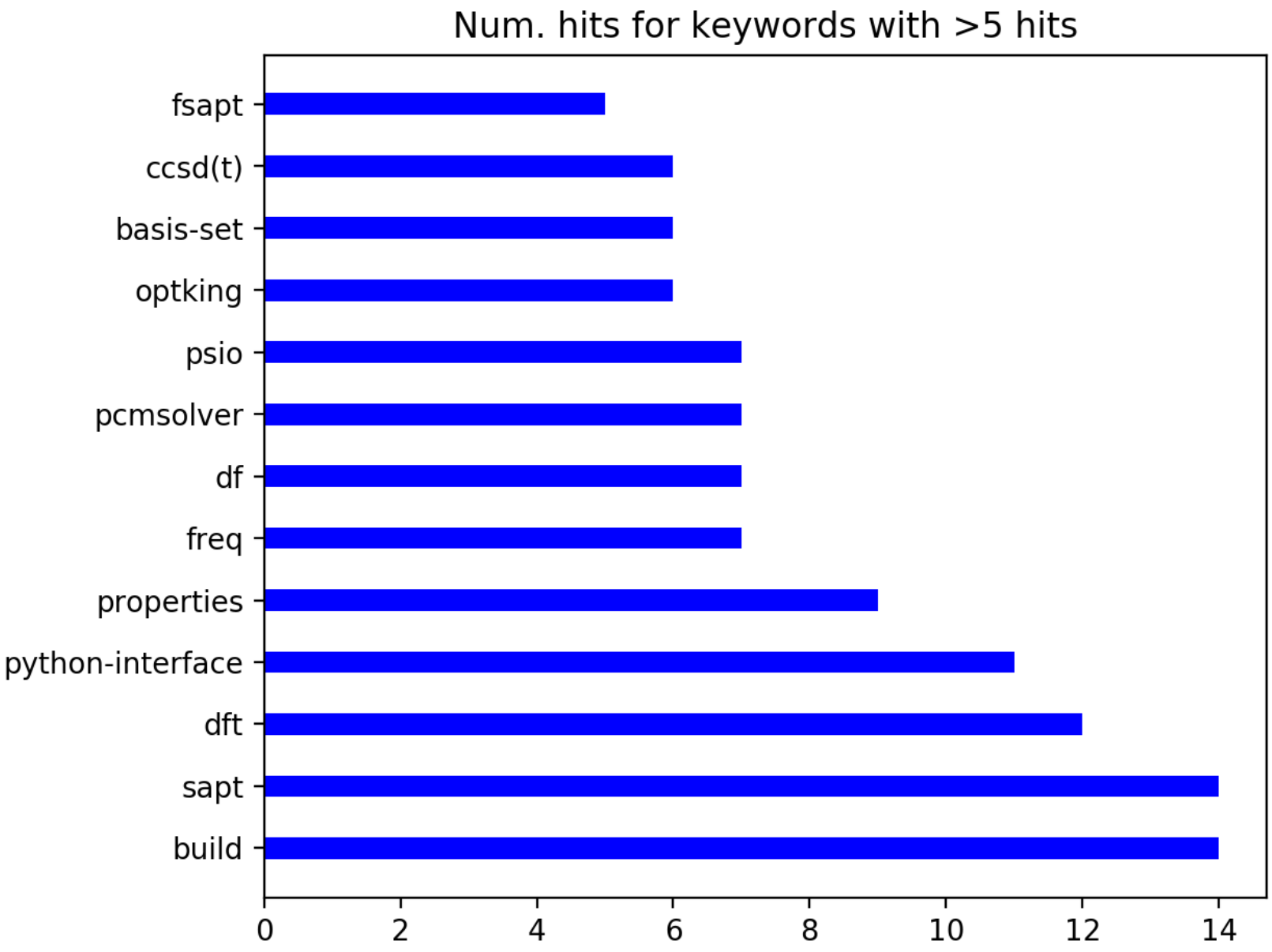
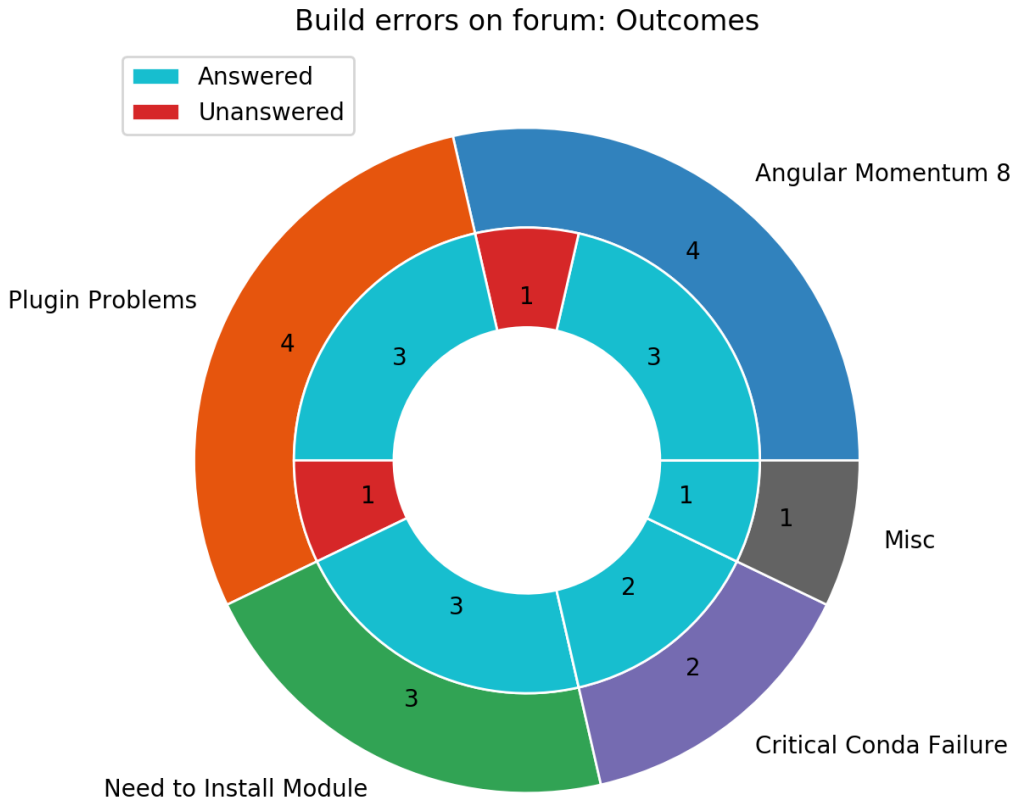
- Forum evidence is ambiguous without addl. context
- Is an issue absent on the forums because it doesn't exist, or because it didn't occur to anybody to ask?
- Do people post about a module because there's a problem with it, or because it sees a lot of use?

What are users posting about?



Public Enemy No. 1: Building

- 14 conversations, 12 topics about build problems



Public Enemy No. 2: PSIO

```
RuntimeError:
Fatal Error: PSIO Error
Error occurred in file: /home/nevensky/.psi4/psi4/psi4/src/psi
```

<input/output files removed>

Thanks for your help.

Reply

created	last reply	2	161	2
N May 29	May 29	replies	views	users

Nevensky May 29

Seems I've ran out of disk space. But the error itself seems obscure at best.

Reply

loriab May 29

Yes, PSIO errors are notoriously unhelpful. We have dreams of switching to hdf5 or bd.

Reply

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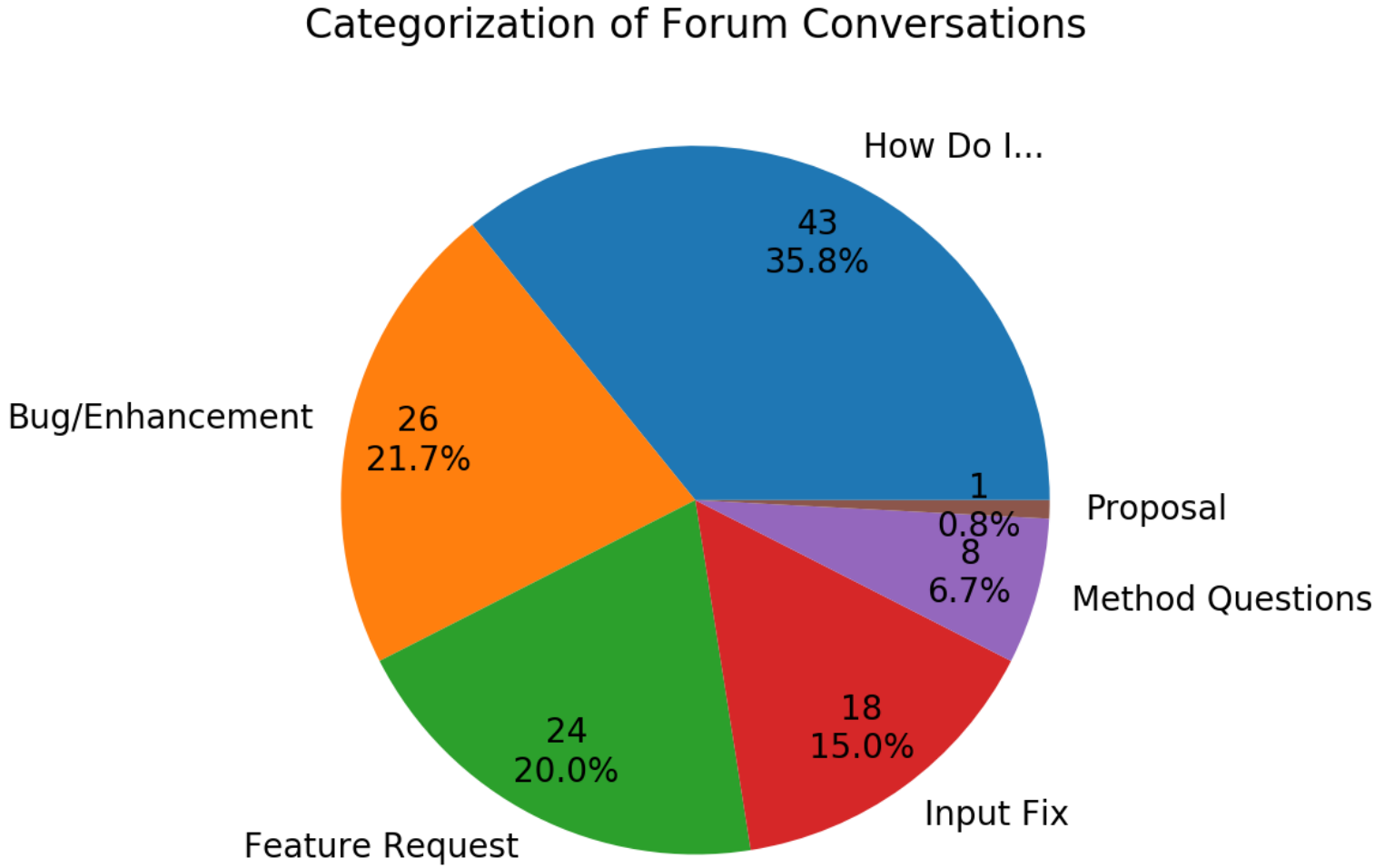
- *dft* has no clear patterns, despite the relatively large sample. Just a common thing to use?


Categorization of Forum Conversations
How Do I...
43
35.8%
Bug/Enhancement
26
21.7%
1
0.8%
Proposal
8
6.7%
Method Questions
18
15.0%
Input Fix
24
20.0%
Feature Request

Proposals

- Timo Strunk proposed a faster way to compute one electron properties. Got a Slack invite the same day. PR accepted.

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- So far, so good!

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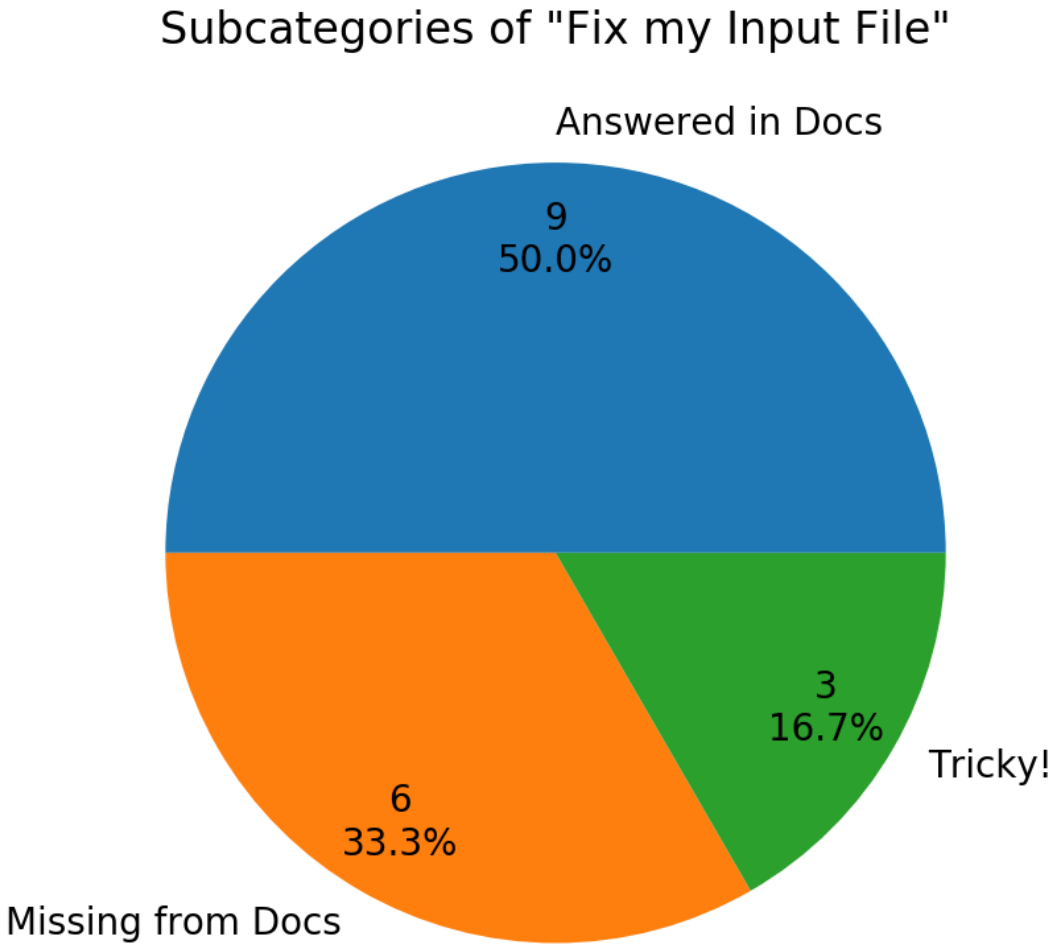
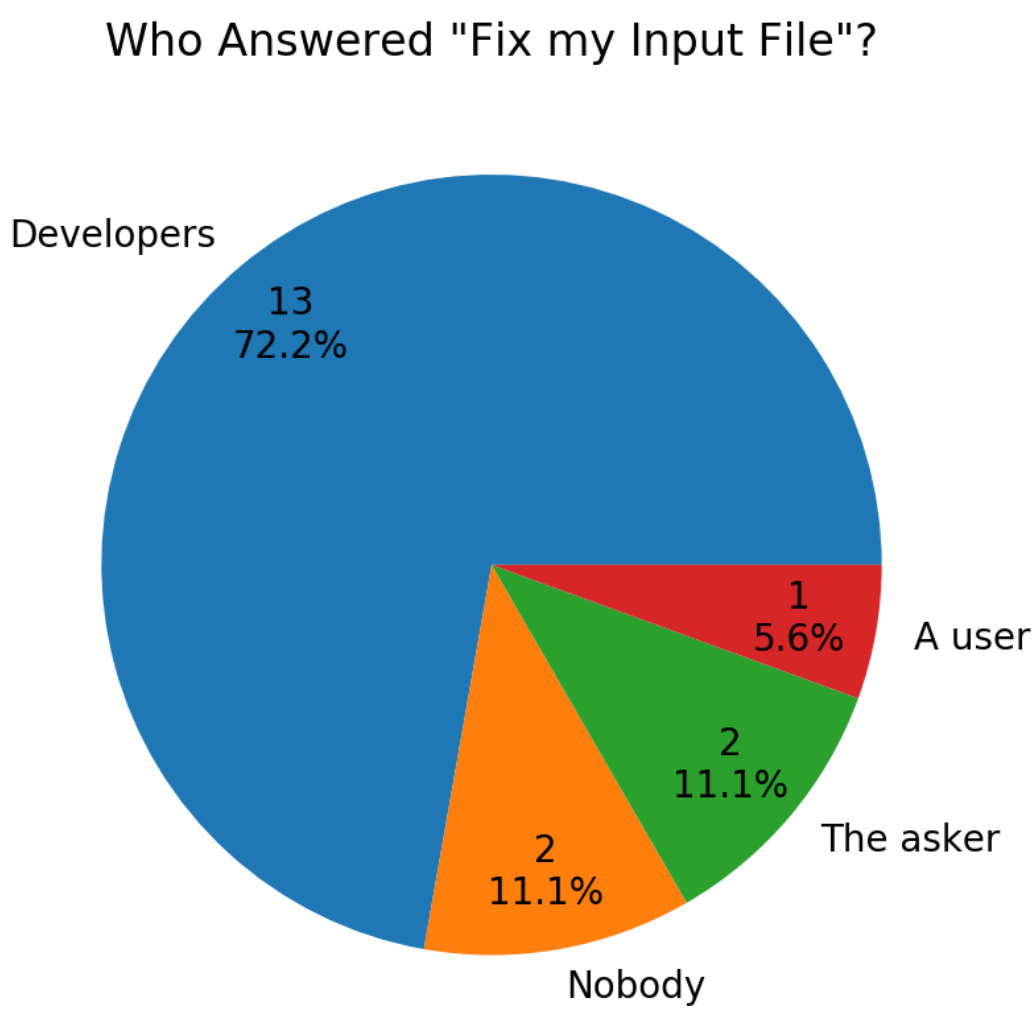
- All answers came from devs


Subcategories of "Fix my Input File"
Answered in Docs
9
50.0%
3
16.7%
Tricky!
6
33.3%
Missing from Docs


Who Answered "Fix my Input File"?
Developers
13
72.2%
1
5.6%
A user
2
11.1%
The asker
2
11.1%
Nobody

What features are being requested?

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- IR intensities, NMR shifts, HOMO/LUMO gradients, DMRG convergence control, ωB97M gradients, exporting multipole integrals, ADC properties, accepting FCHK files as input, estimating job memory, wavefunction serialization, 3 body SAPT, SCF level shifting, TDDFT, more customization of frozen core commands, easier "embedding potentials", cube files for valence electrons, ωB97M(2), more readable timer data...

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- The forum is no help in prioritizing these

What features have we fulfilled?

1. More readable timer data

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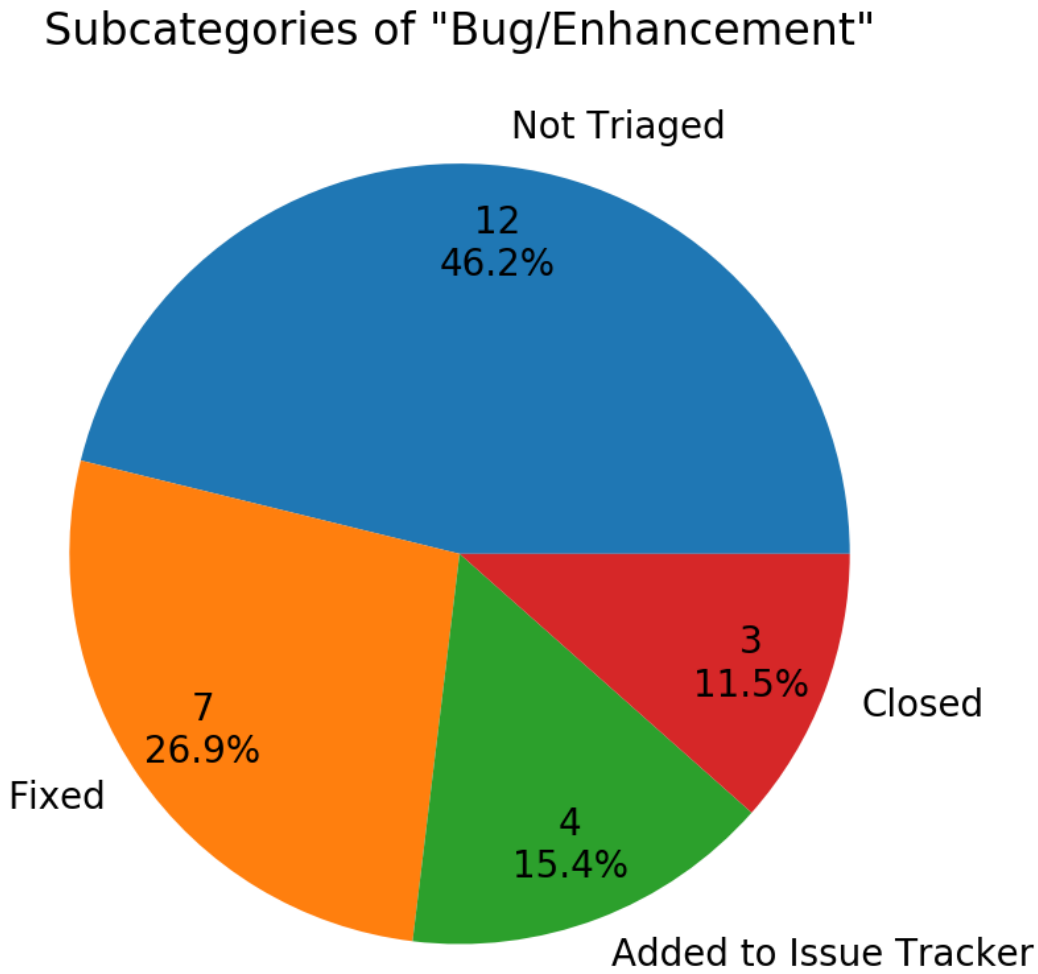
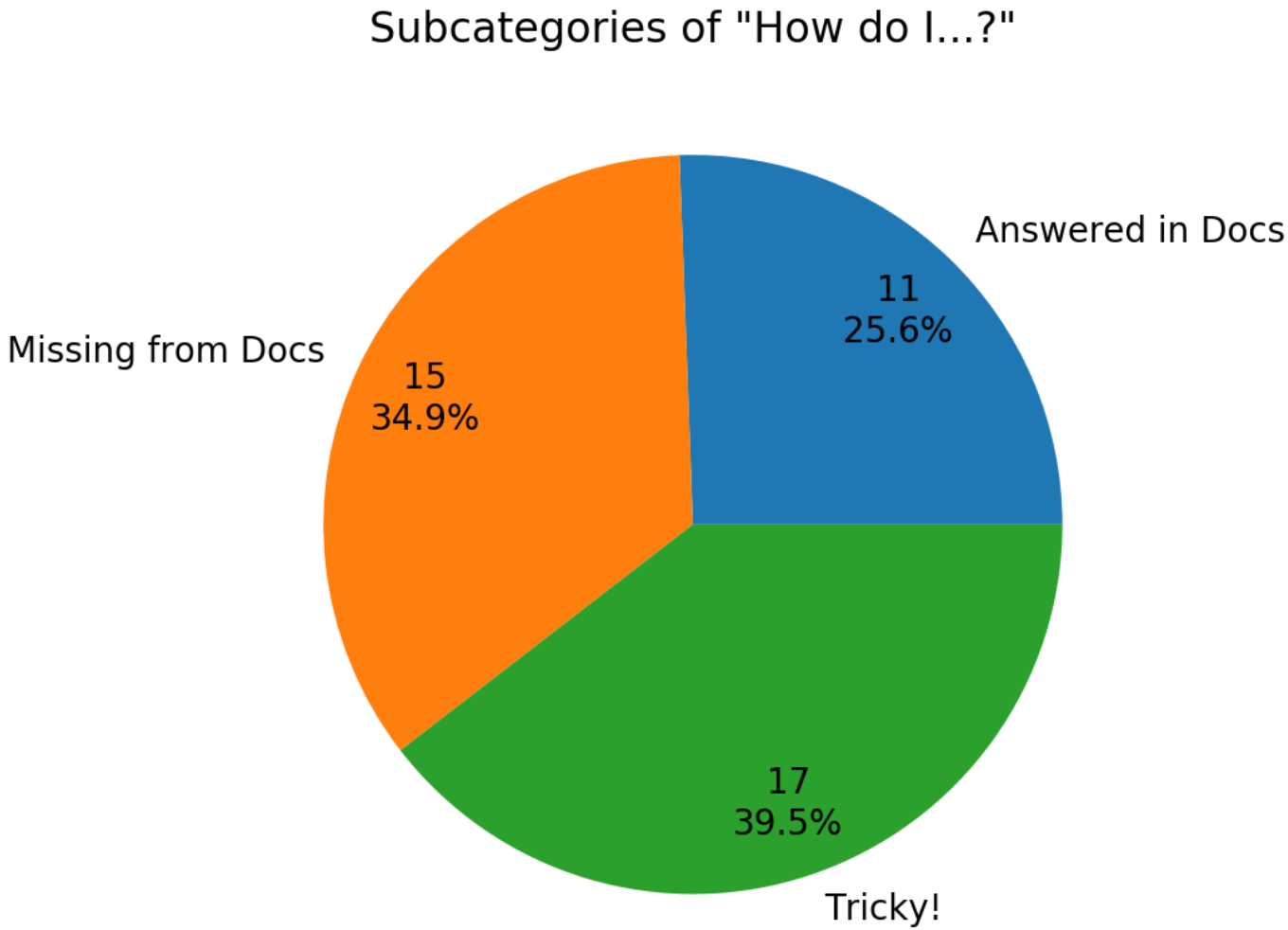
- Only the timer readability influenced dev decisions


Subcategories of "Bug/Enhancement"
Not Triaged
12
46.2%
3
11.5%
Closed
7
26.9%
Fixed
4
15.4%
Added to Issue Tracker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11
25.6%
Missing from Docs
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34.9%
17
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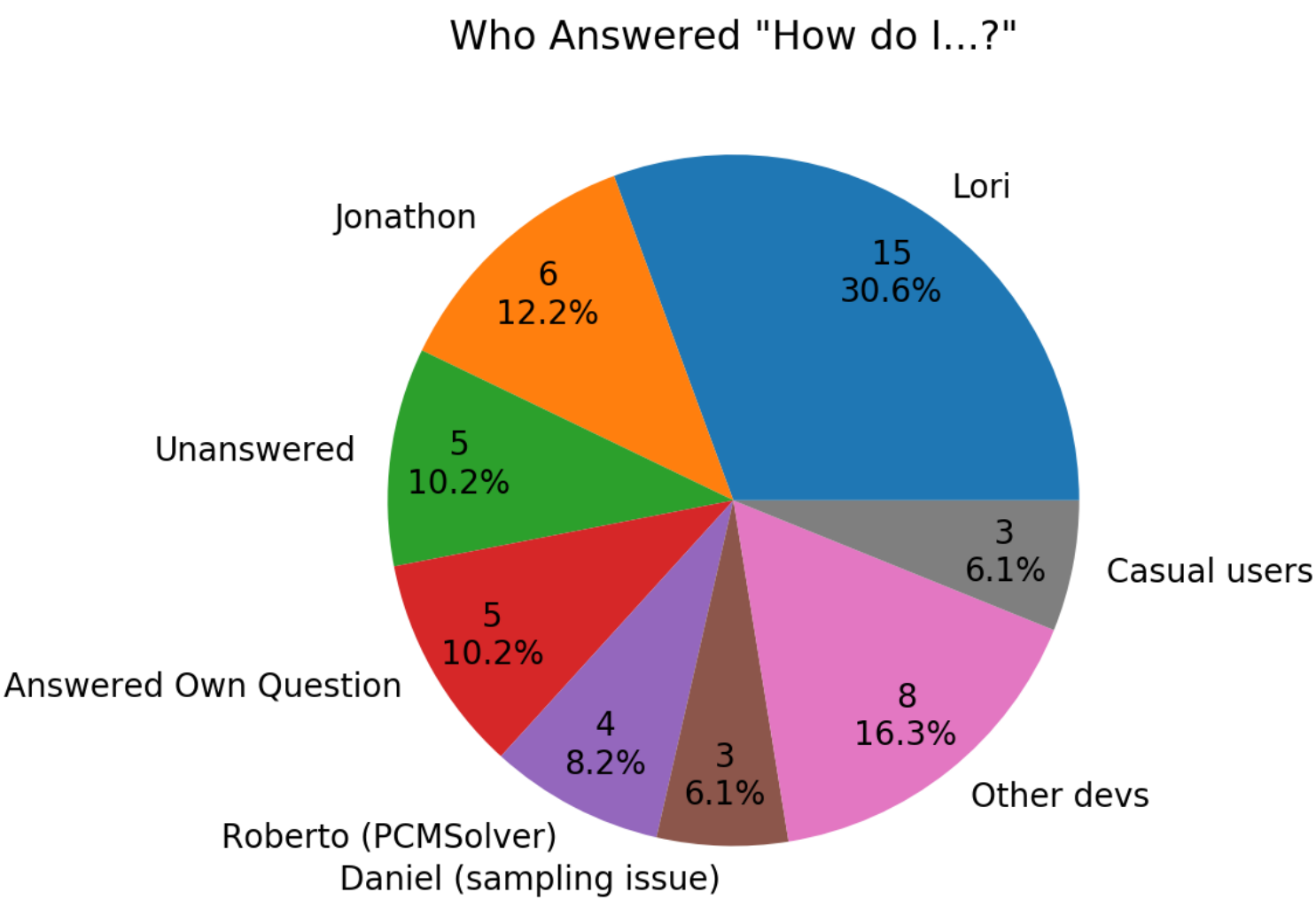
Who Answered "How do I...?"
Lori
15
30.6%
Jonathon
6
12.2%
Unanswered
5
10.2%
Answered Own Question
5
10.2%
Roberto (PCMSolver)
4
8.2%
Daniel (sampling issue)
3
6.1%
Other devs
8
16.3%
Casual users
3
6.1%