Getting Scientific Software Installed
Tools & Best Practices

... AND WE HAVE A SPECIAL INSURANCE OVER $100,000,000 FOR THE CASE THAT SOMETHING HAPPENS TO JIM

WOW! THAT'S A LOT FOR A CEO

CEO? HE'S THE GUY WHO UNDERSTANDS OUR BUILD SCRIPTS

HOW TO BECOME INVALUABLE

ISC'14 Birds-of-a-Feather session
June 24th 2014

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HPC-UGent in a nutshell

- HPC team at central IT dept. of Ghent University (Belgium)
  - 9 team members: 1 manager, ~3 user support, ~5 sysadmin
  - 6 Tier2 clusters + one Tier1 (8.5k cores), ~1k servers in total
  - ~1.2k user accounts, all research domains
  - tasks incl. hardware, system administration, user support/training, …
- member of Flemish Supercomputer Centre (VSC)
  - virtual centre, collaboration between Flemish university associations

ISC'14 BoF session
Getting Scientific Software Installed
Tools & Best Practices
Outline

- lightning talks

    - **HPC Advisory Council** (Pak Lui, HPC Advisory Council)

    - **Lmod** (Robert McLay, TACC)

    - **EasyBuild** (Jens Timmerman, UGent)

- **show-of-hands** and a couple of key topics

- **open discussion**

    - what are the major issues (for you)?

    - which tools are you using, and would you recommend?

Show of hands (setup)

- Go to **socrative.com**

    (use your laptop, smartphone, tablet, ...)

- Click 'Student Login'

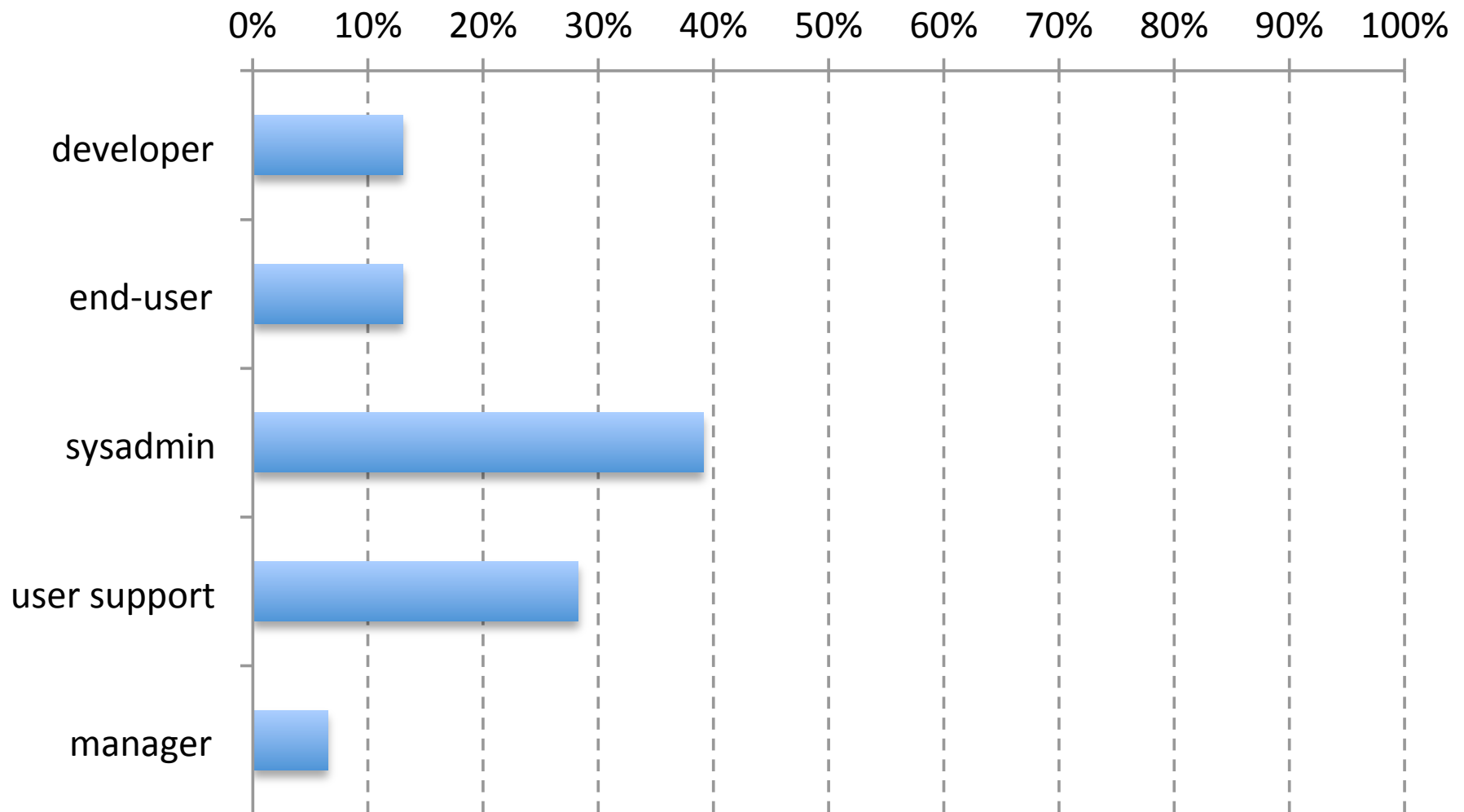- Enter the room number: **570181**

- Participate!

Who are you?

SC13 BoF
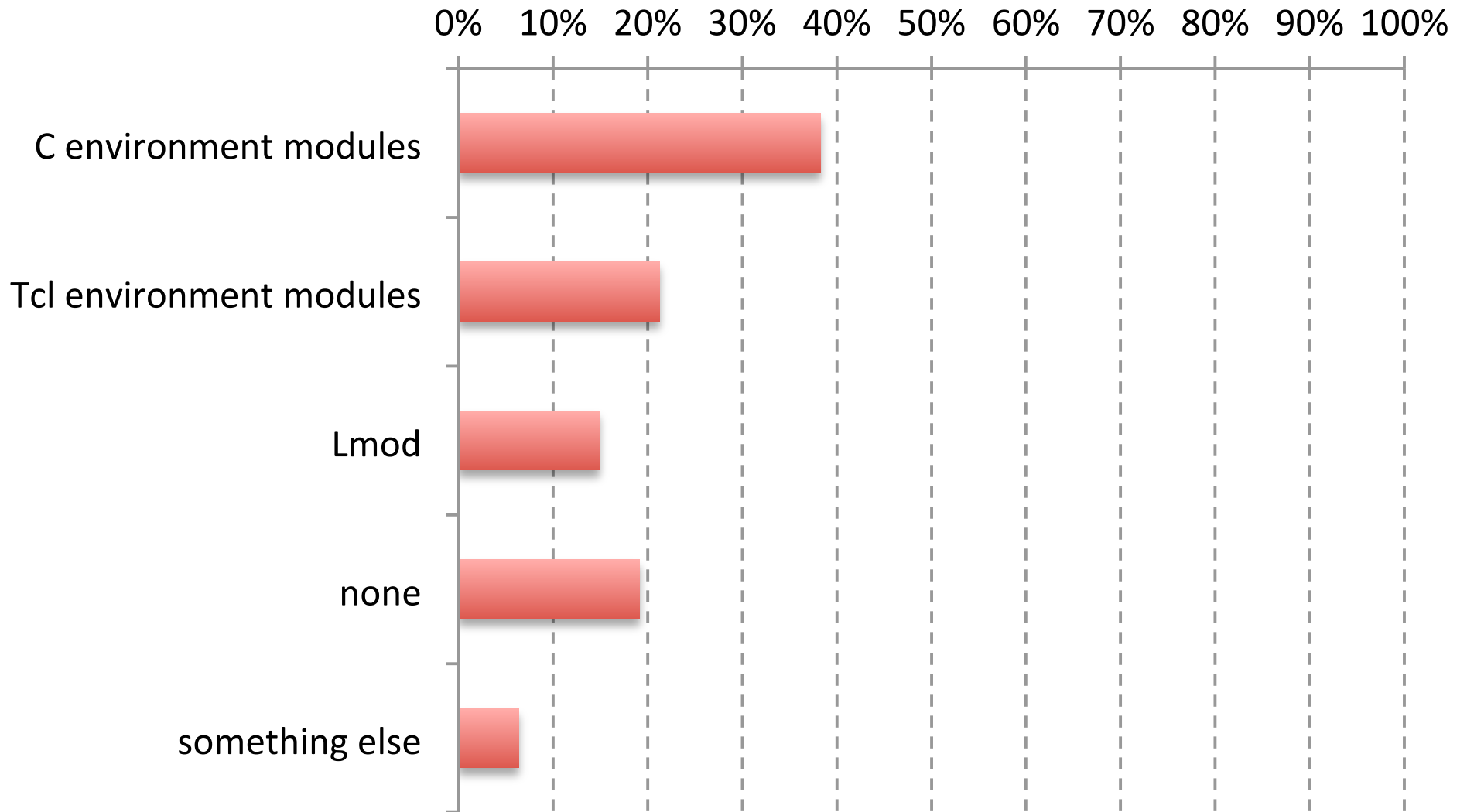**Getting Scientific Software Installed: Tools & Best Practices**
Who are you? (46)

Which modules tool do you use?

SC13 BoF
Getting Scientific Software Installed: Tools & Best Practices
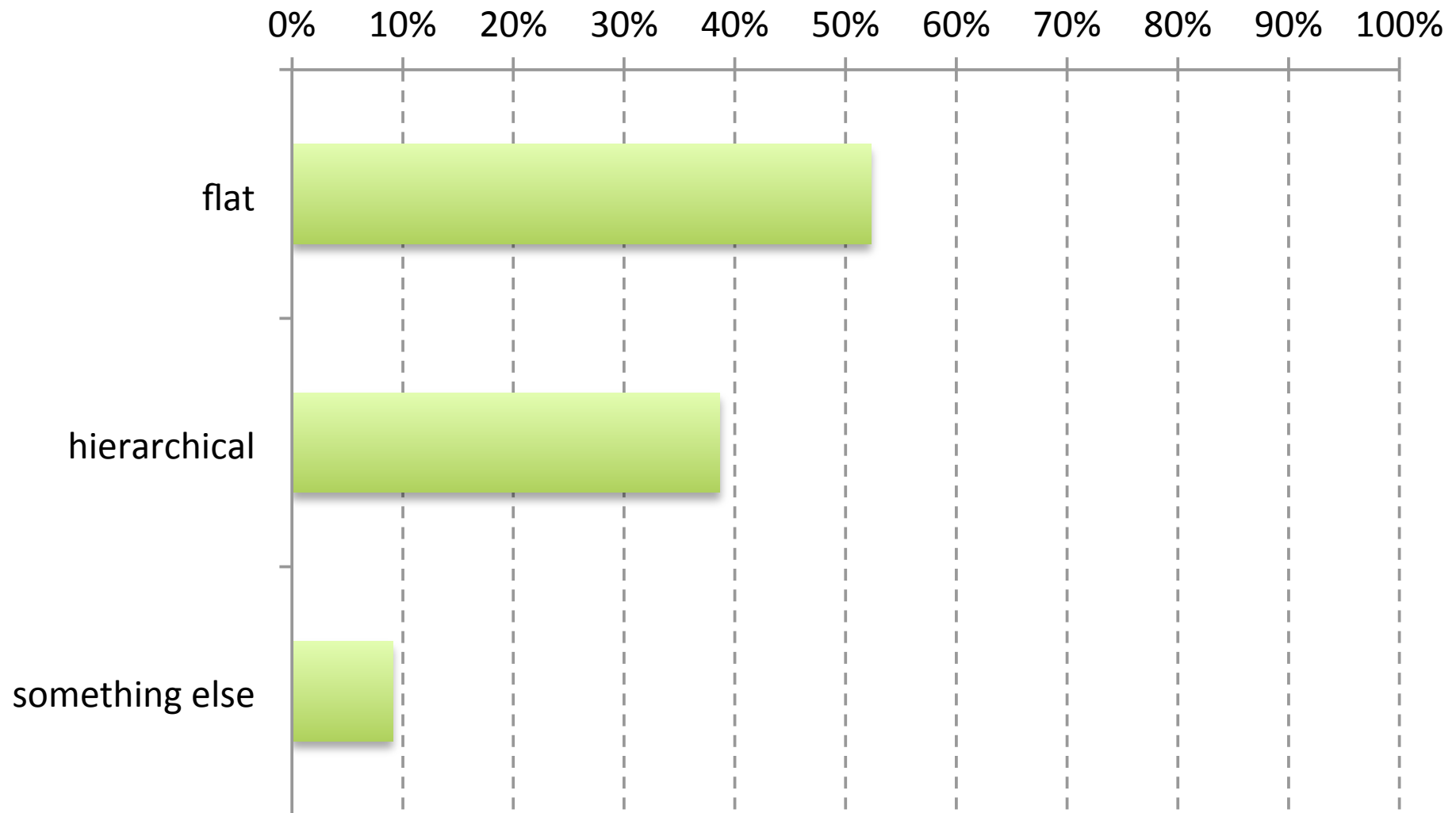**Which modules tool do you use? (47)**

Which module naming scheme do you use?

SC13 BoF
Getting Scientific Software Installed: Tools & Best Practices
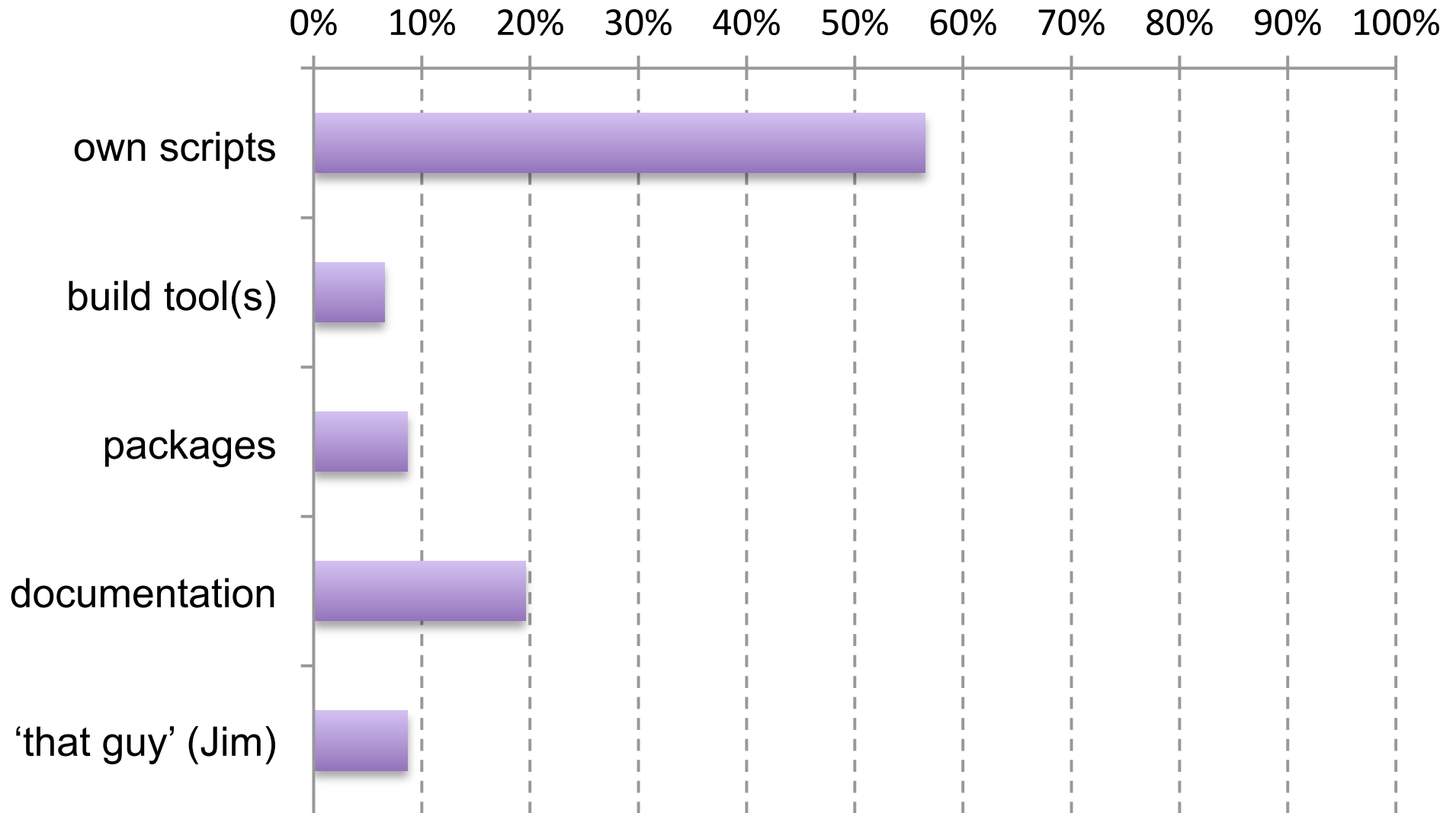**Which modules naming scheme do you use? (44)**

Tools for building/installing scientific software

SC13 BoF
Getting Scientific Software Installed: Tools & Best Practices
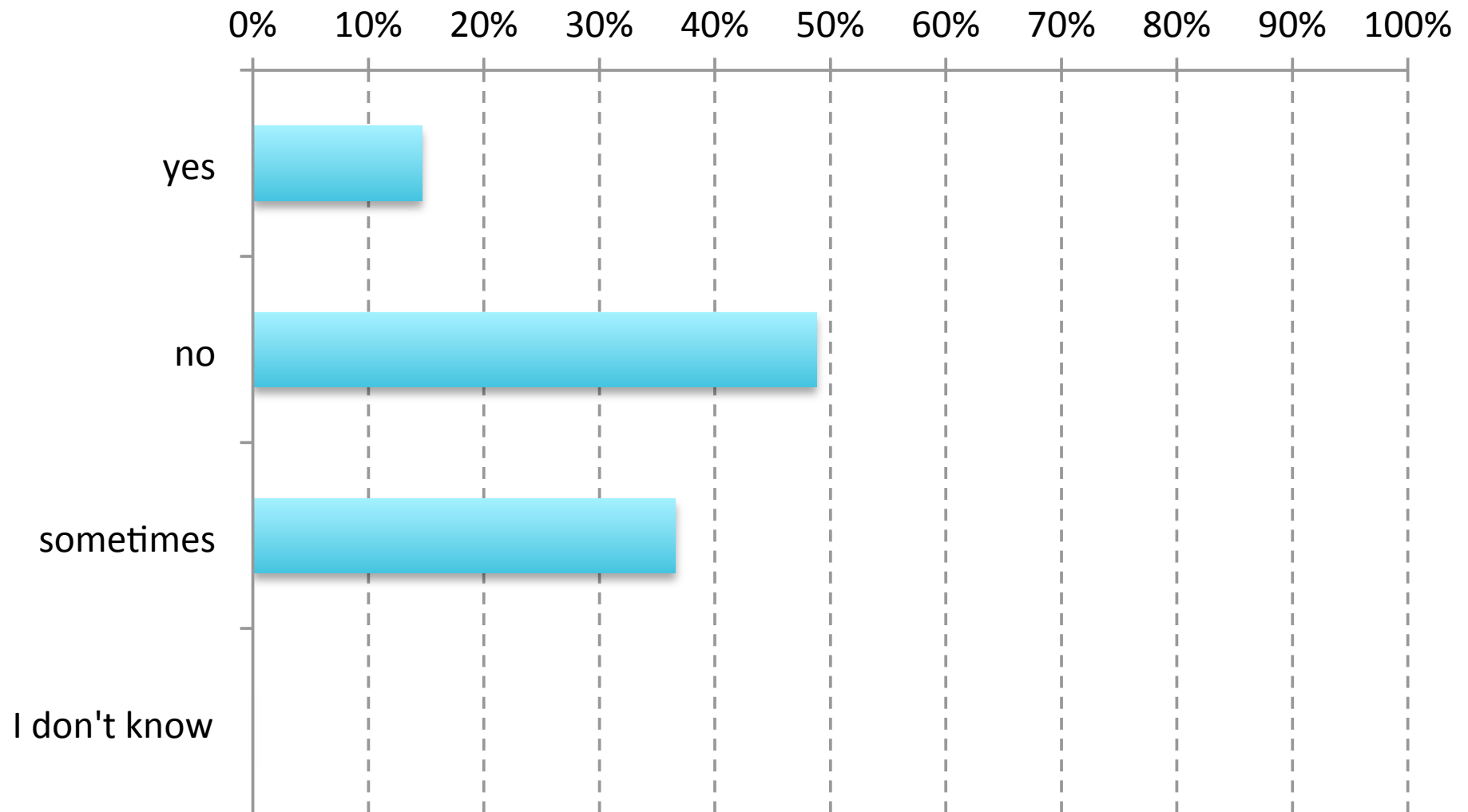**How do you build and install software?** (46)

Best practices, which ones do you use?

SC13 BoF

Getting Scientific Software Installed: Tools & Best Practices

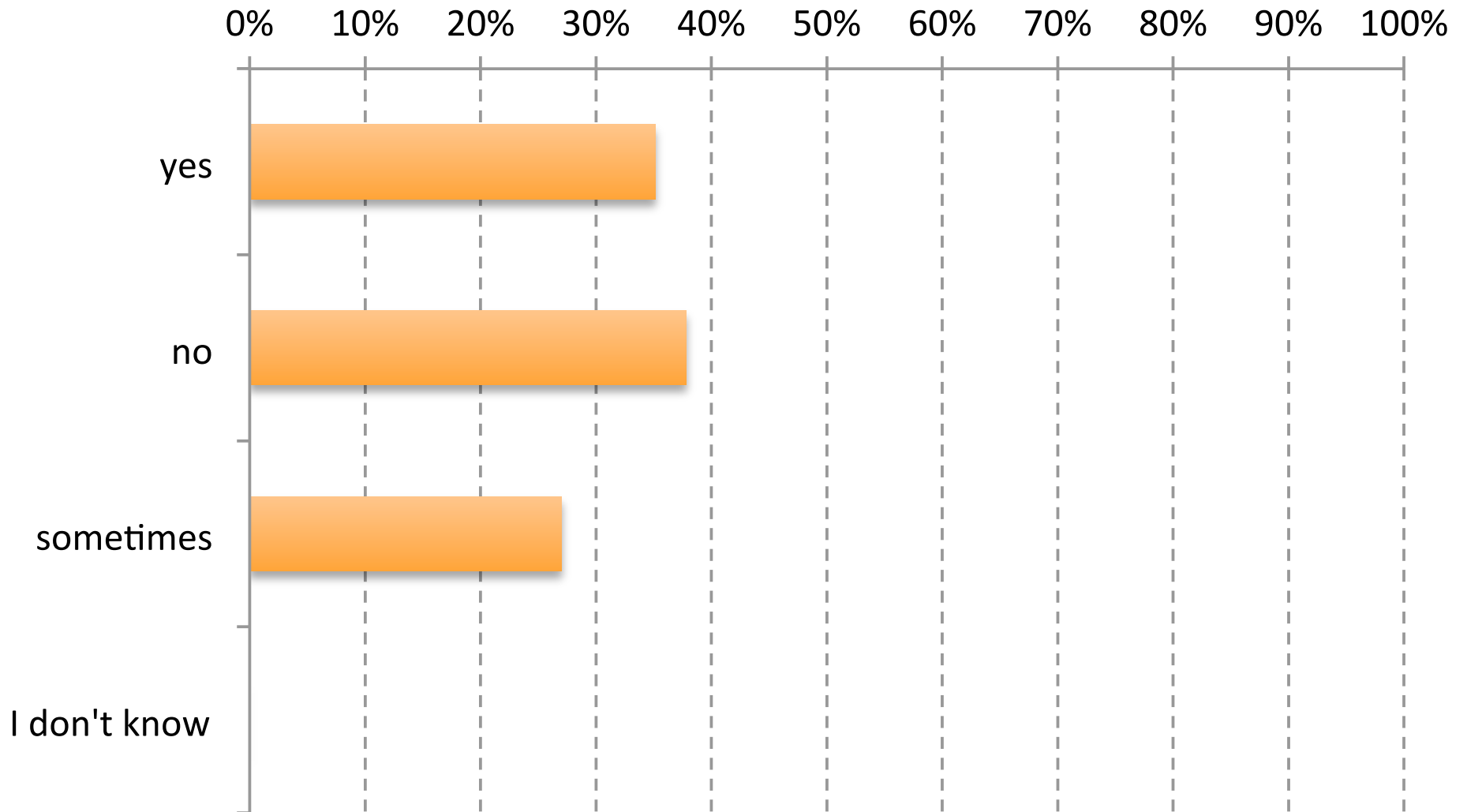**Do you collaborate with other sites?** (41)

Best practices, which ones do you use?

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Getting Scientific Software Installed: Tools & Best Practices
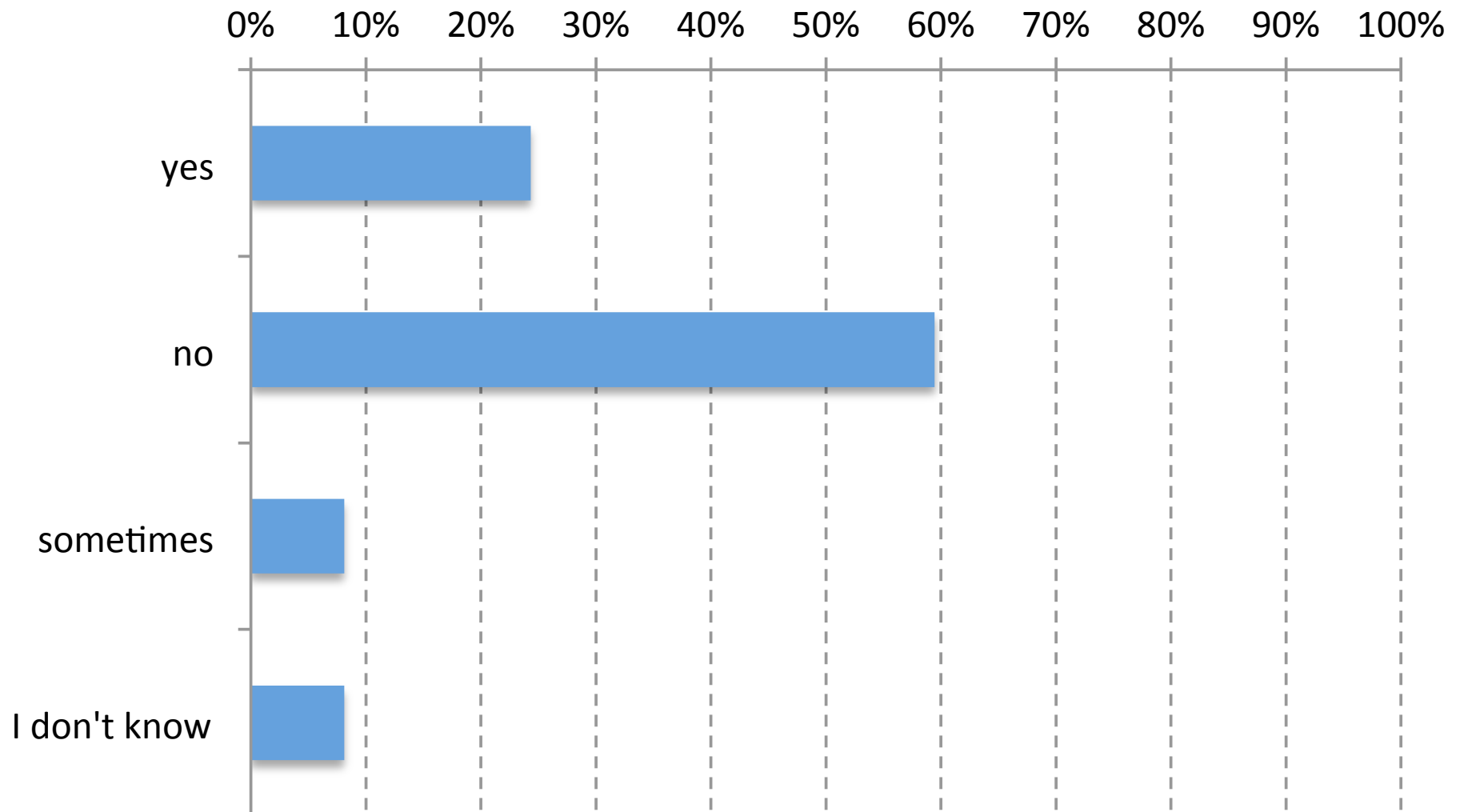**Do you automate software builds? (37)**

Best practices, which ones do you use?

SC13 BoF
Getting Scientific Software Installed: Tools & Best Practices
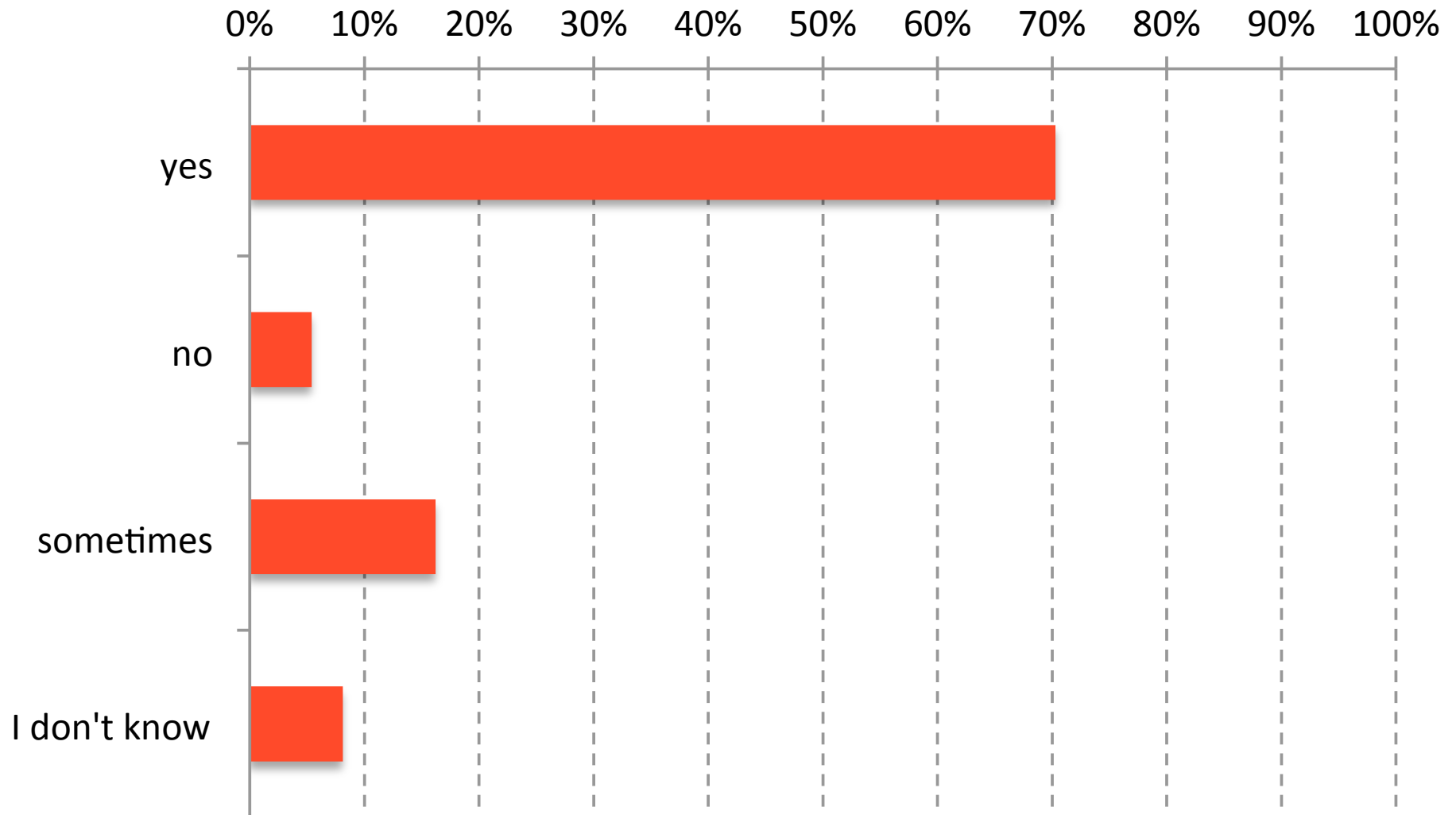**Are module files generated automatically? (37)**

Best practices, which ones do you use?

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Getting Scientific Software Installed: Tools & Best Practices
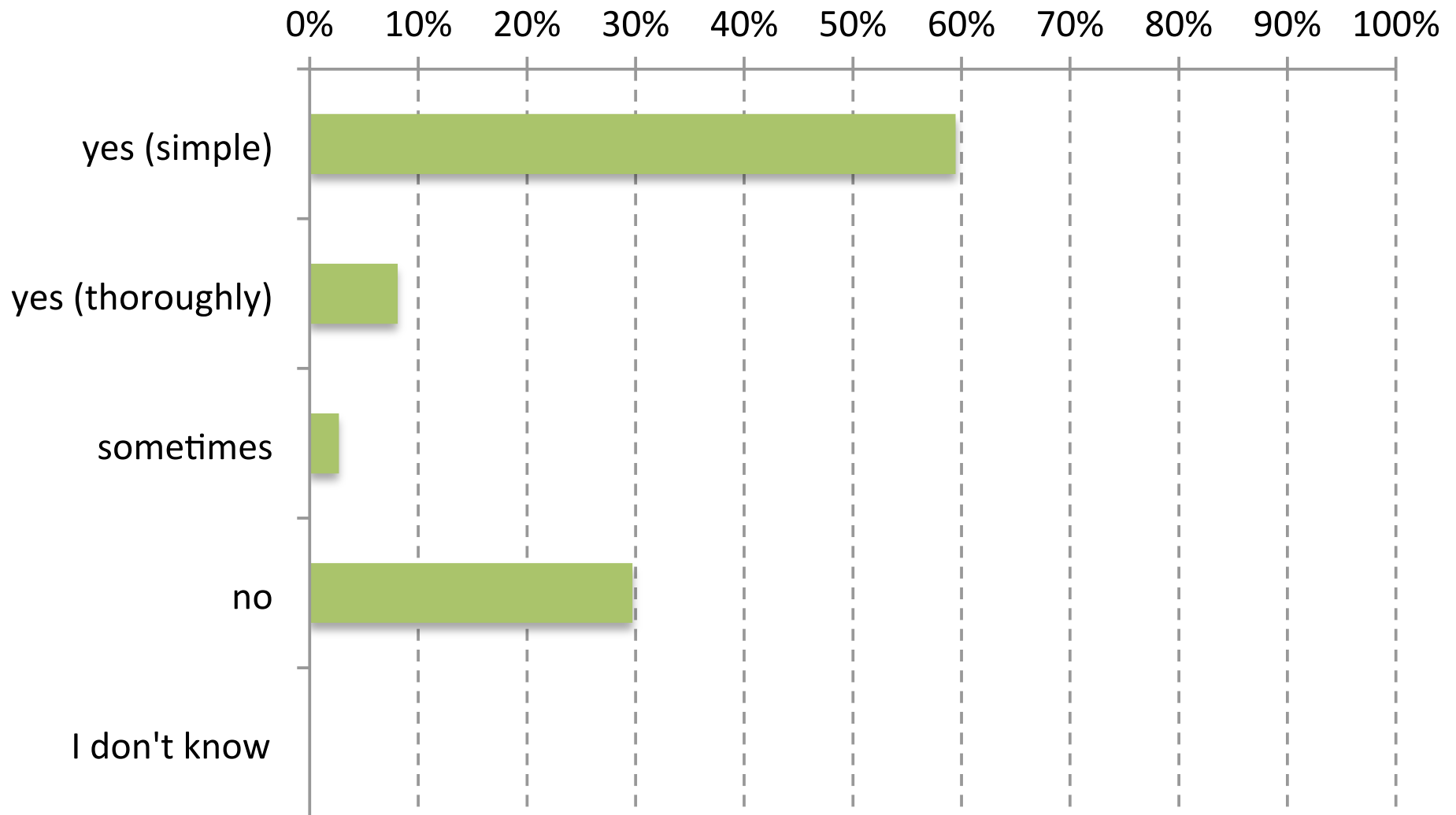**Do you provide multiple builds per application? (37)**

Best practices, which ones do you use?

SC13 BoF
Getting Scientific Software Installed: Tools & Best Practices
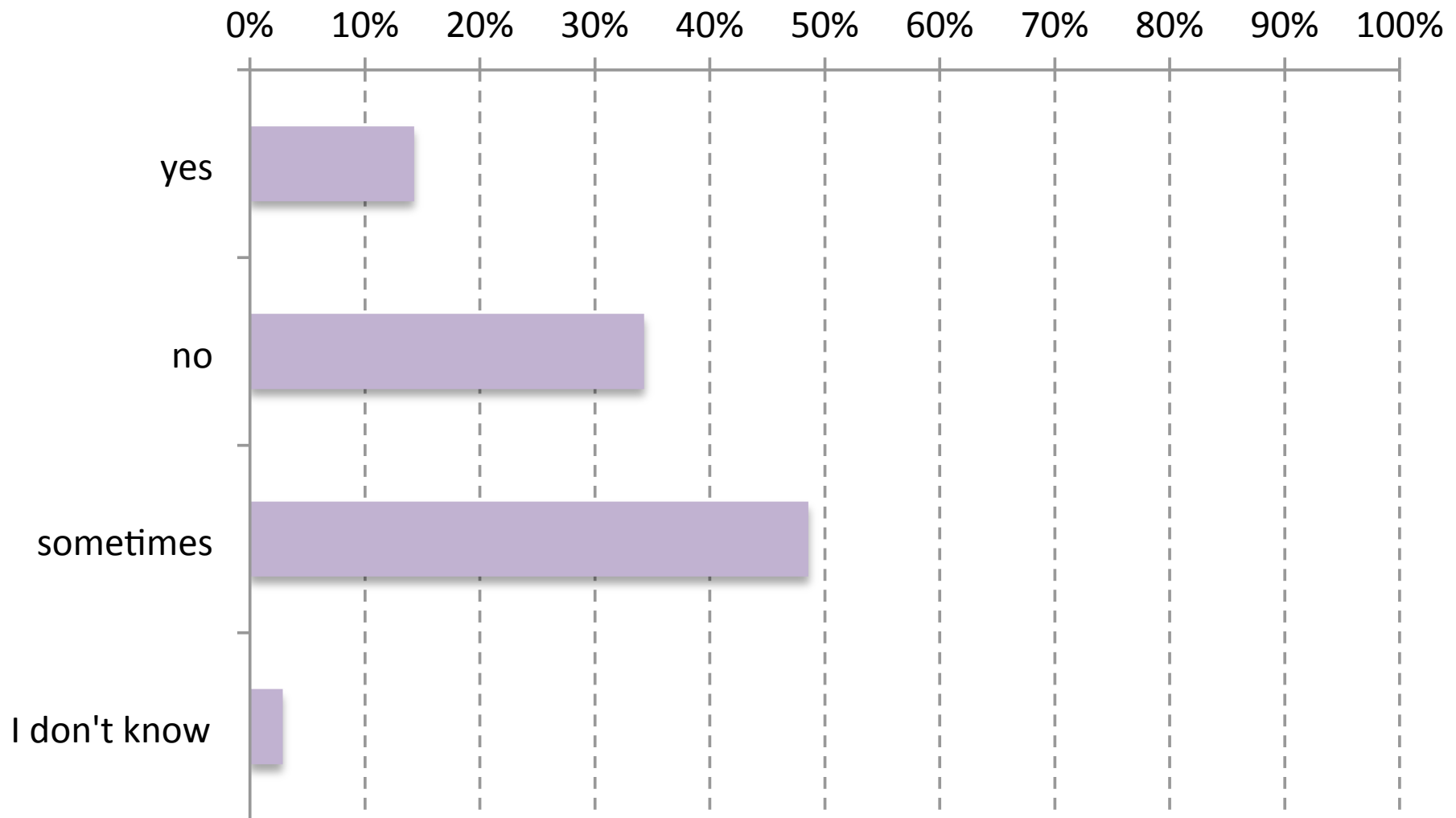**Do you test the software builds (correctness)? (37)**

Best practices, which ones do you use?

SC13 BoF
Getting Scientific Software Installed: Tools & Best Practices
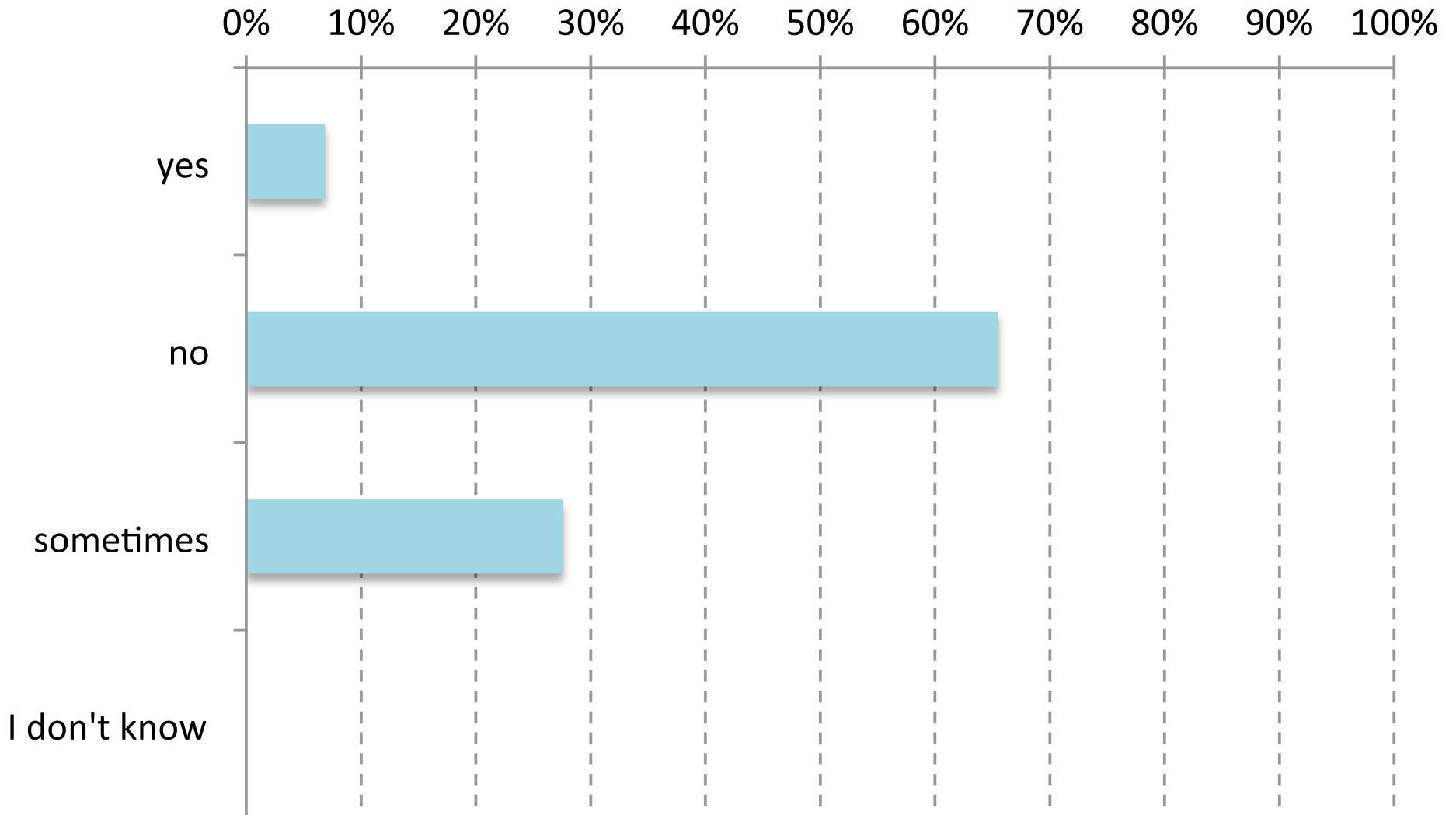**Do you evaluate performance of the software? (35)**

Best practices, which ones do you use?

SC13 BoF
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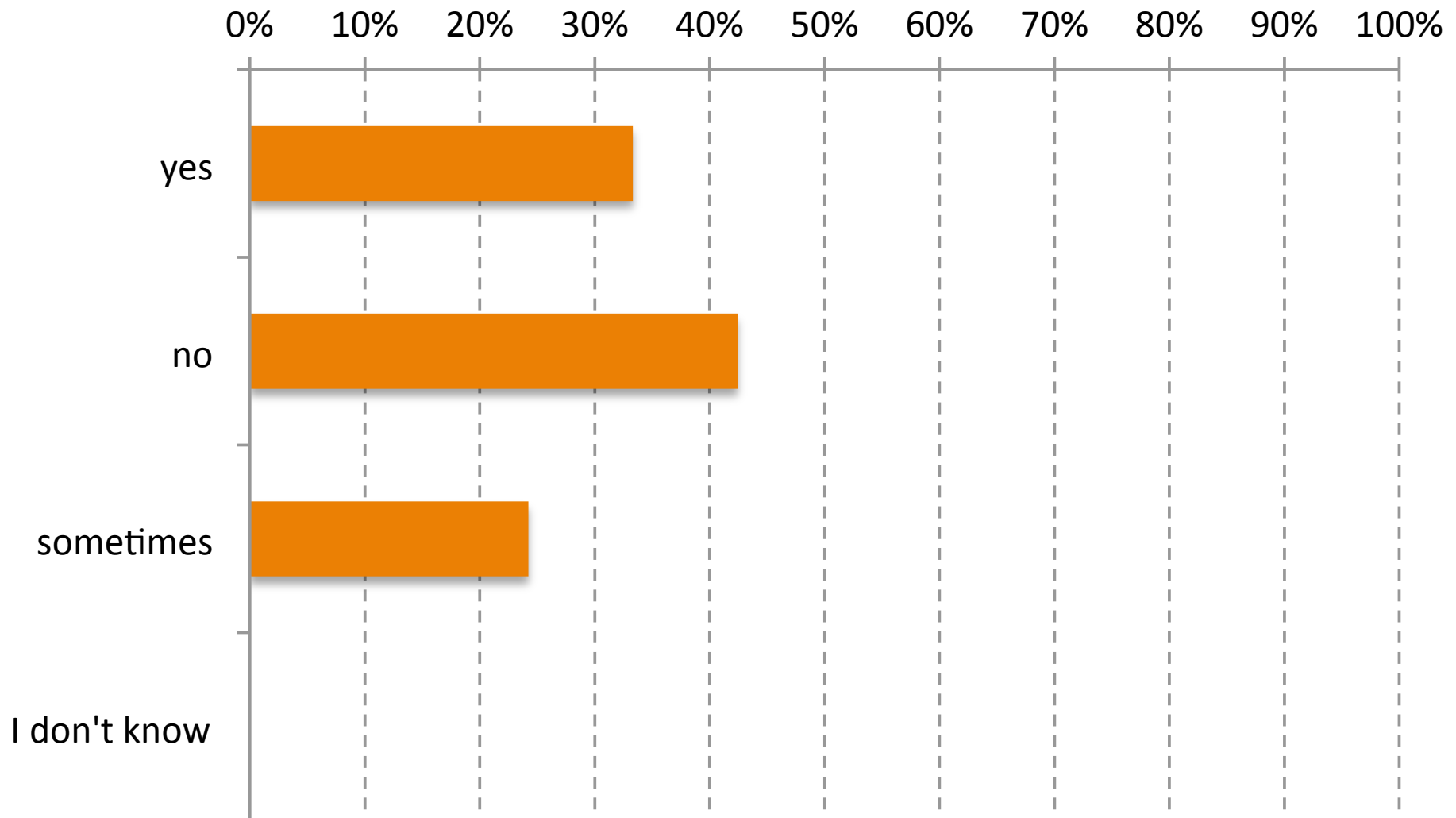**Do you monitor performance of the software? (29)**

Best practices, which ones do you use?

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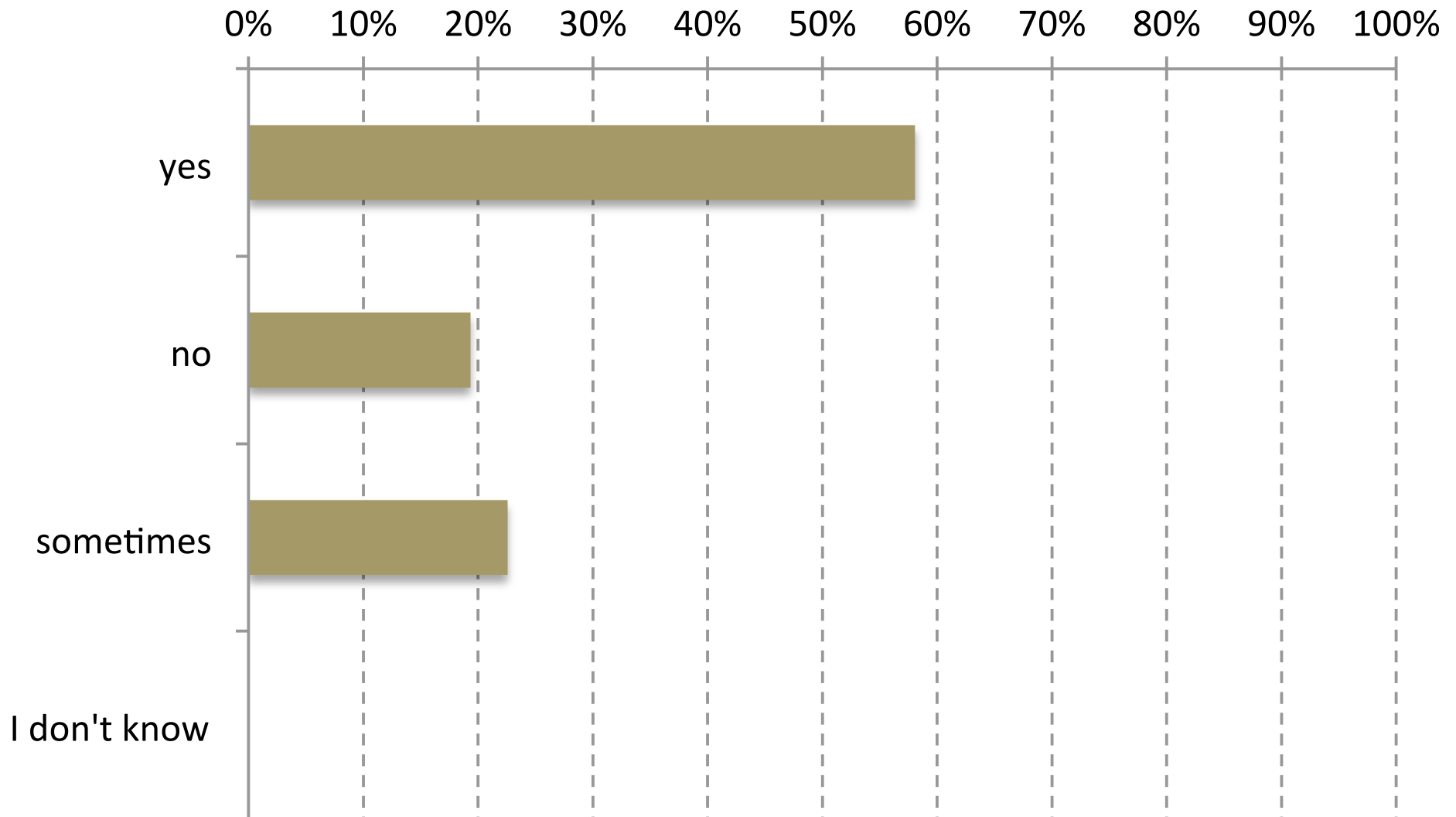**Do you keep track of build metadata? (33)**

16
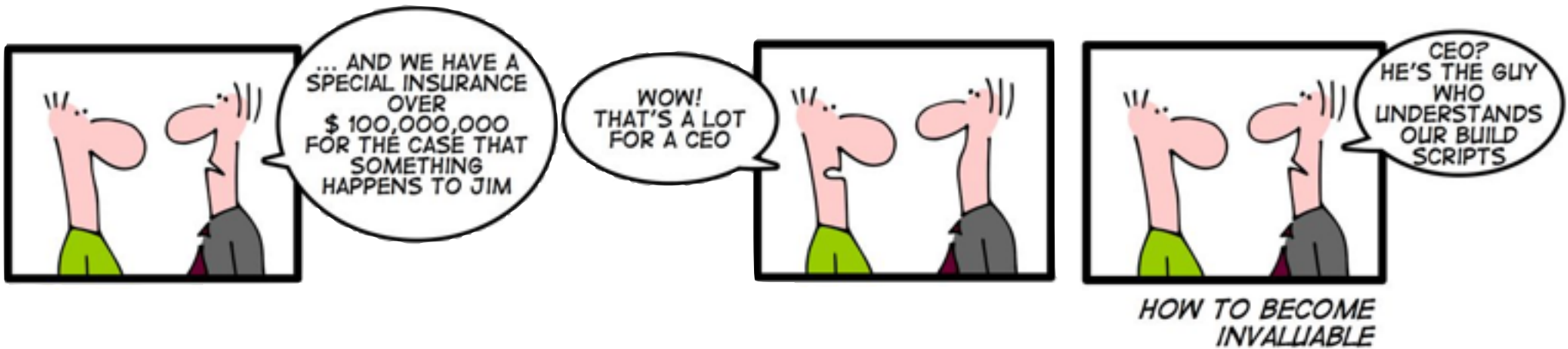
Best practices. which ones do you use?

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Do you keep an archive of software sources? (31)

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http://geekandpoke.typepad.com/geekandpoke/2010/05/how-to-become-invaluable.html