LIBECPINT: OPEN SOURCE SOFTWARE

ROBERT SHAW

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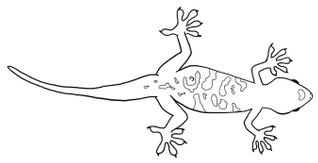
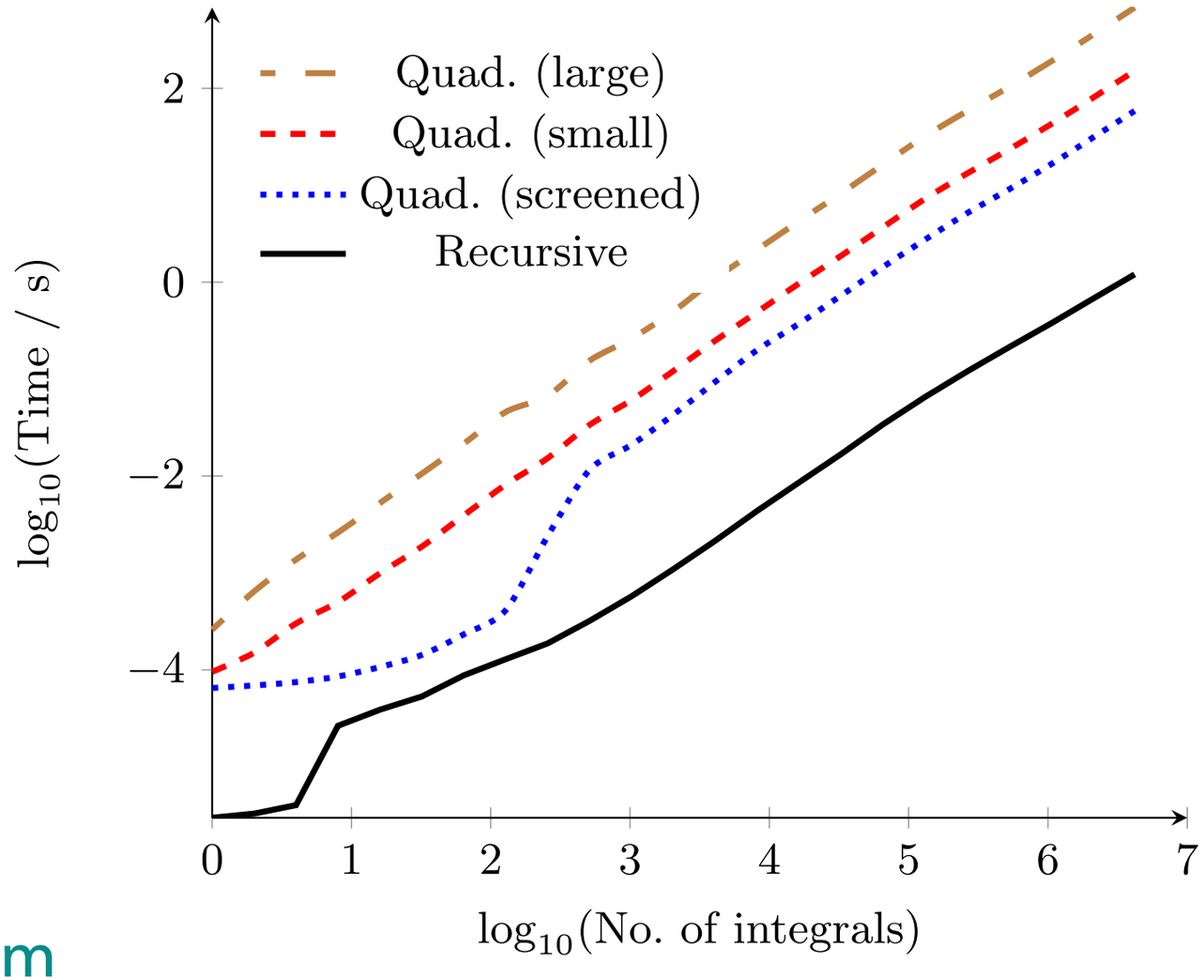


WHAT IS LIBECPINT?

- Fast, robust calculation of integrals over effective core potentials
- Open source C++ library
  - Extensible
  - Reproducible
  - Lightweight
- Now used by several quantum chemistry packages



[1] RA Shaw, JG Hill, *JCP*, 2017, **147** (7), 074108
[2] RA Shaw, JG Hill, *JOSS*, 2021, **6** (60)

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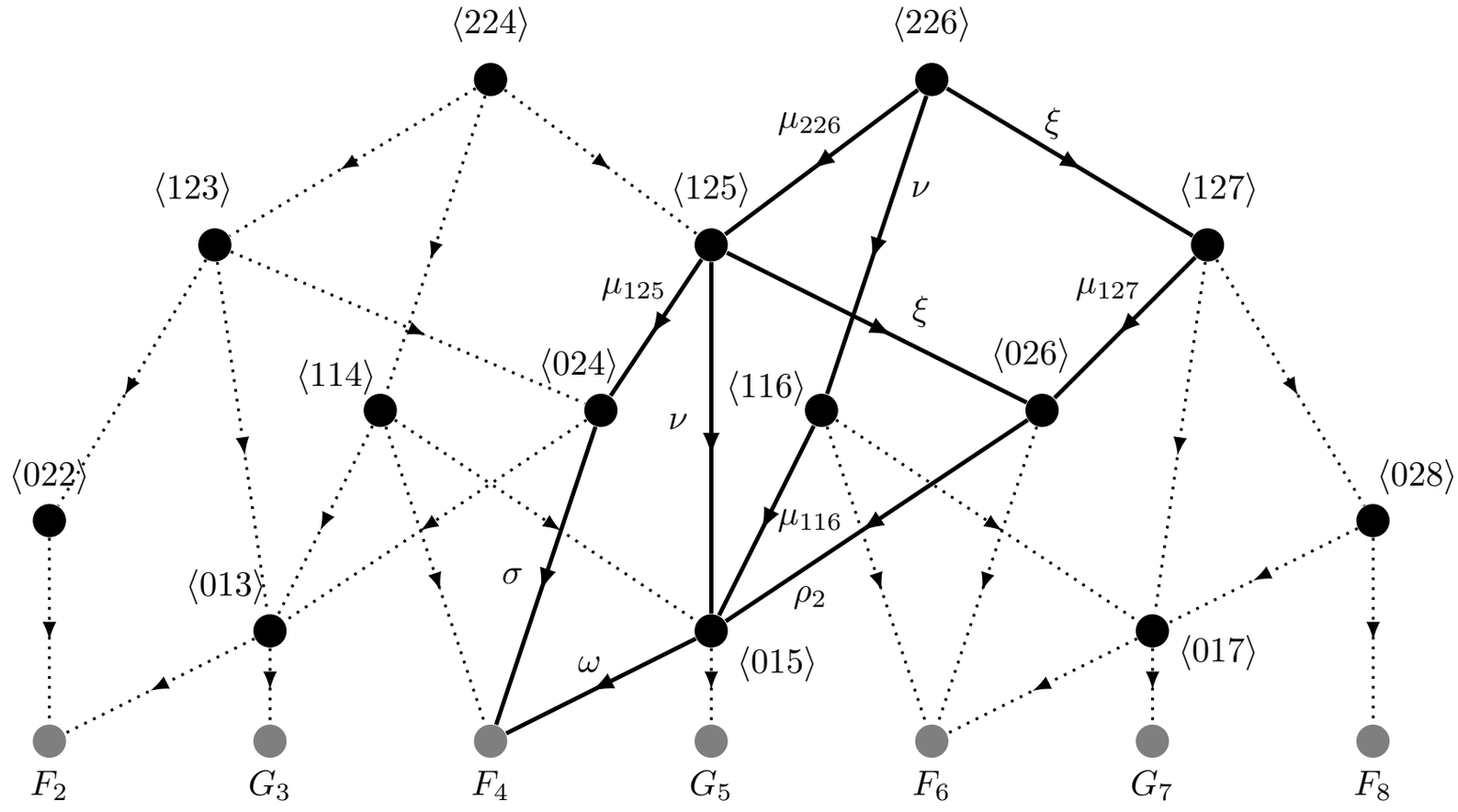
WHY IS IT NEEDED?

- Electronic integrals are complicated
- ECPs have significant benefits
  - Efficiency
  - Accuracy
- Avoid people reinventing the wheel



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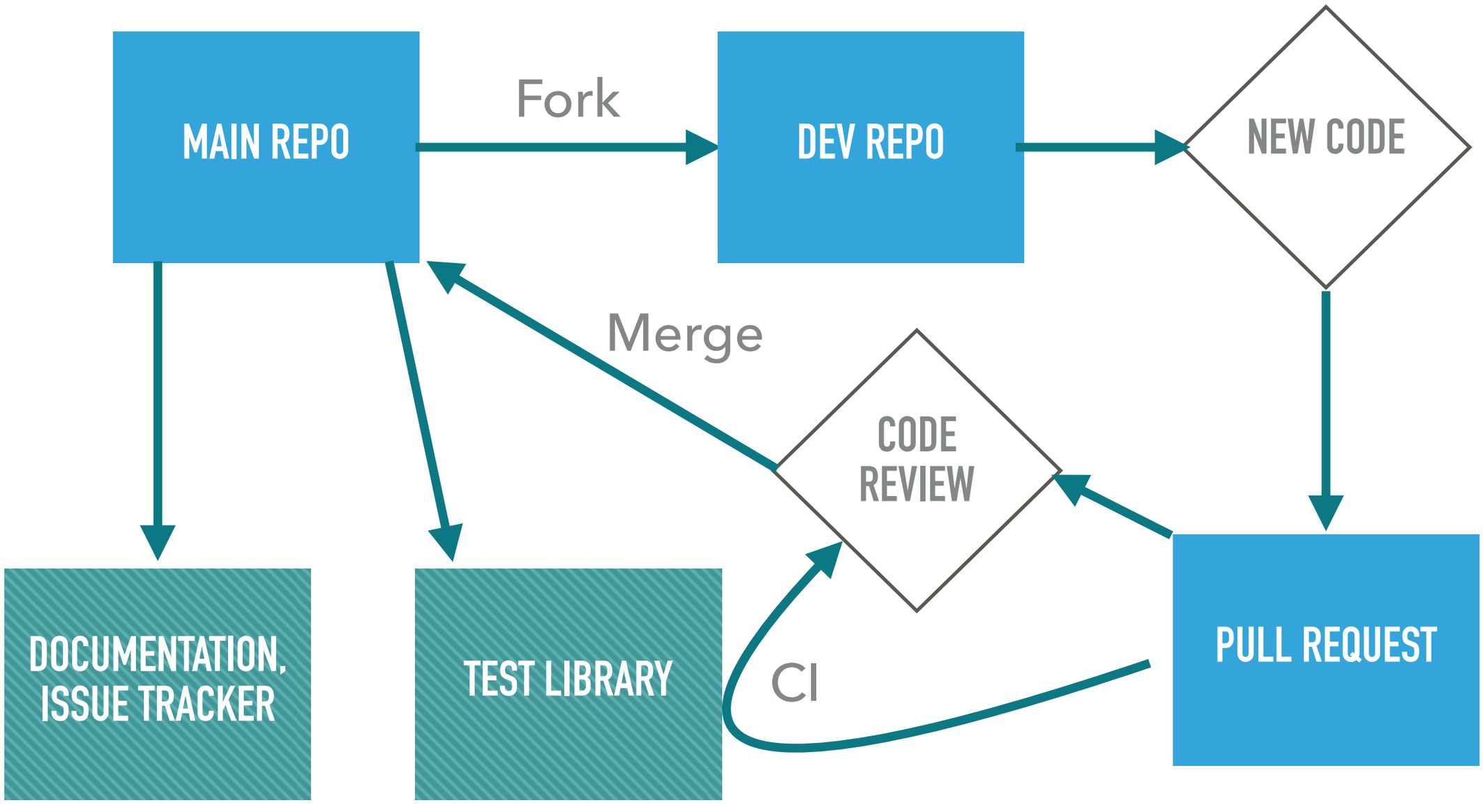
OPEN SOURCE DEVELOPMENT



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JOURNAL OF OPEN SOURCE SOFTWARE

JOSS
The Journal of Open Source Software

libecpint: A C++ library for the efficient evaluation of integrals over effective core potentials

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Software

- Review
- Repository
- Archive

Summary

Effective core potentials (ECPs) are widely-used in computational chemistry both to reduce the computational cost of calculations (M. Dolg, 2000) and include relevant physics that

Software repository
Paper review
Download paper
Software archive

Review

Editor: @poulson (all papers)
Reviewers: @felipeZ (all reviews), @lorenzo-rovigatti (all reviews)

Authors

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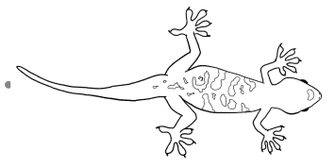

LEARNINGS

- A lot of (largely thankless) work and effort
  - Extra work at the beginning, saves a lot of time later
- Absolutely worth it:
  - Code is easier to maintain
  - Future-proofed
  - Easily citable
- Essential for future of computational science

OSS at: www.github.com/robashaw

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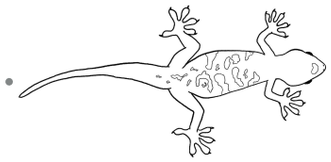

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