Lazy matrices for contraction-based algorithms

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UNIVERSITÄT HEIDELBERG
ZUKUNFT SEIT 1386

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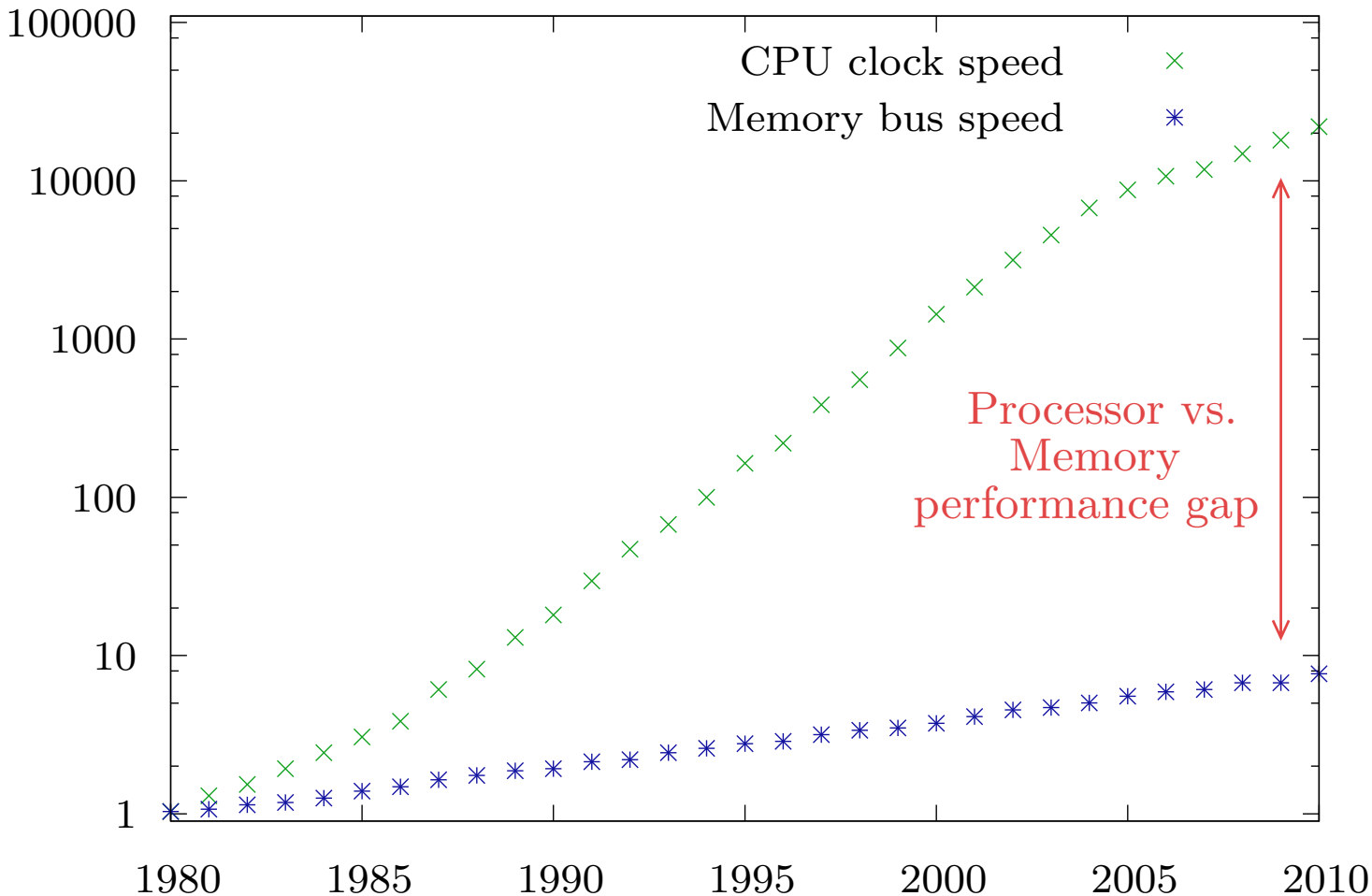
Processor vs. memory performance improvement



Data from `https://dave.cheney.net/2014/06/07/five-things-that-make-go-fast`

Hartree-Fock equations

- Hartree-Fock equations

$$\left(-\frac{1}{2}\Delta + \hat{\mathcal{V}}_{\text{Nuc}} + \hat{\mathcal{V}}_{\text{H}}\left[\{\psi_f\}_{f\in I}\right] + \hat{\mathcal{V}}_{\text{x}}\left[\{\psi_f\}_{f\in I}\right] - \varepsilon_f\right)\psi_f(\underline{\boldsymbol{r}}) = 0$$

with

$-\frac{1}{2}\Delta$	Kinetic energy of electrons
$\hat{\mathcal{V}}_{\text{Nuc}}$	Electron-nuclear interaction
$\hat{\mathcal{V}}_{\text{H}}\left[\{\psi_f\}_{f\in I}\right]$	Hartree potential
$\hat{\mathcal{V}}_{\text{x}}\left[\{\psi_f\}_{f\in I}\right]$	Exchange potential

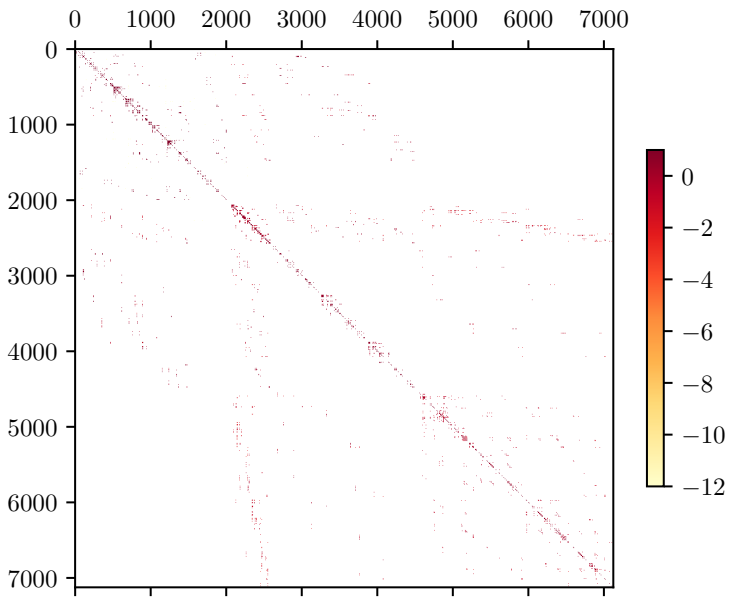
- Non-linear system of partial differential equations
- Non-linear eigenproblem for eigenpairs $\{(\varepsilon_f, \psi_f)\}_{f\in I}$

Finite-element discretisation

- Finite elements: Piecewise polynomials with support only on a few neighbouring *cells*

$\Rightarrow$ Need many finite elements ($> 10^6$)

- Typically sparse matrix structures:

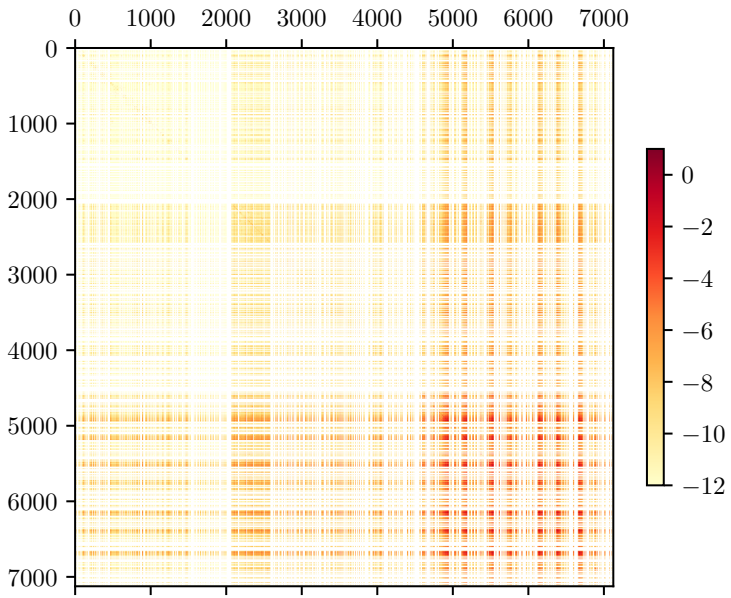


Typical discretisation of $-\frac{1}{2}\Delta + \hat{\mathcal{V}}_{\mathrm{Nuc}} + \hat{\mathcal{V}}_{\mathrm{H}}$

Finite-element discretisation

Caveat

- But … $\hat{\mathcal{V}}_{\mathrm{x}}$ is so-called *non-local*:



K: Discretisation of $\hat{\mathcal{V}}_{\mathrm{x}}$

- Building **K** takes $\Omega(N^2)$ time and $\mathcal{O}(N^2)$ storage
- Typically $10^6 \cdot 10^6$ elements $\approx 8\,\mathrm{TB}$ storage

Finite-element discretisation

contraction-based scheme

- Iterative solvers only need matrix-vector products
- Matrix-vector product of $\mathbf{K}$: Theoretically $\mathcal{O}(N)$

$\Rightarrow$ contraction-based or matrix-free algorithm:

- Never build $\mathbf{K}$ in storage
- Use expression for $\mathbf{K}$ to directly form contraction of matrix to vectors

contraction-based SCF

Possible problems

- For SCF we will need

$$\mathbf{F} = \mathbf{T} + \mathbf{V}_{\mathrm{Nuc}} + \mathbf{J} + \mathbf{K} + \cdots$$

- Requirements differ:
  - Optimal storage scheme
  - Optimal contraction scheme
  - Approximations / costs

$\Rightarrow$ `contraction` expression complicated to code

$\Rightarrow$ We would like to stay flexible

Characteristics of `contraction`-based algorithms

Advantages

- Scaling (storage and time) reduced — in examples to $\mathcal{O}(N)$
- Parallelisation easier
  - $\Rightarrow$ Less data management
- Hardware trends are in favour

Disadvantages

- Matrices more intuitive than `contraction`-functions
- More computations
  - $\Rightarrow$ Need efficient contraction schemes for the `contraction`
  - $\Rightarrow$ Algorithms more complicated

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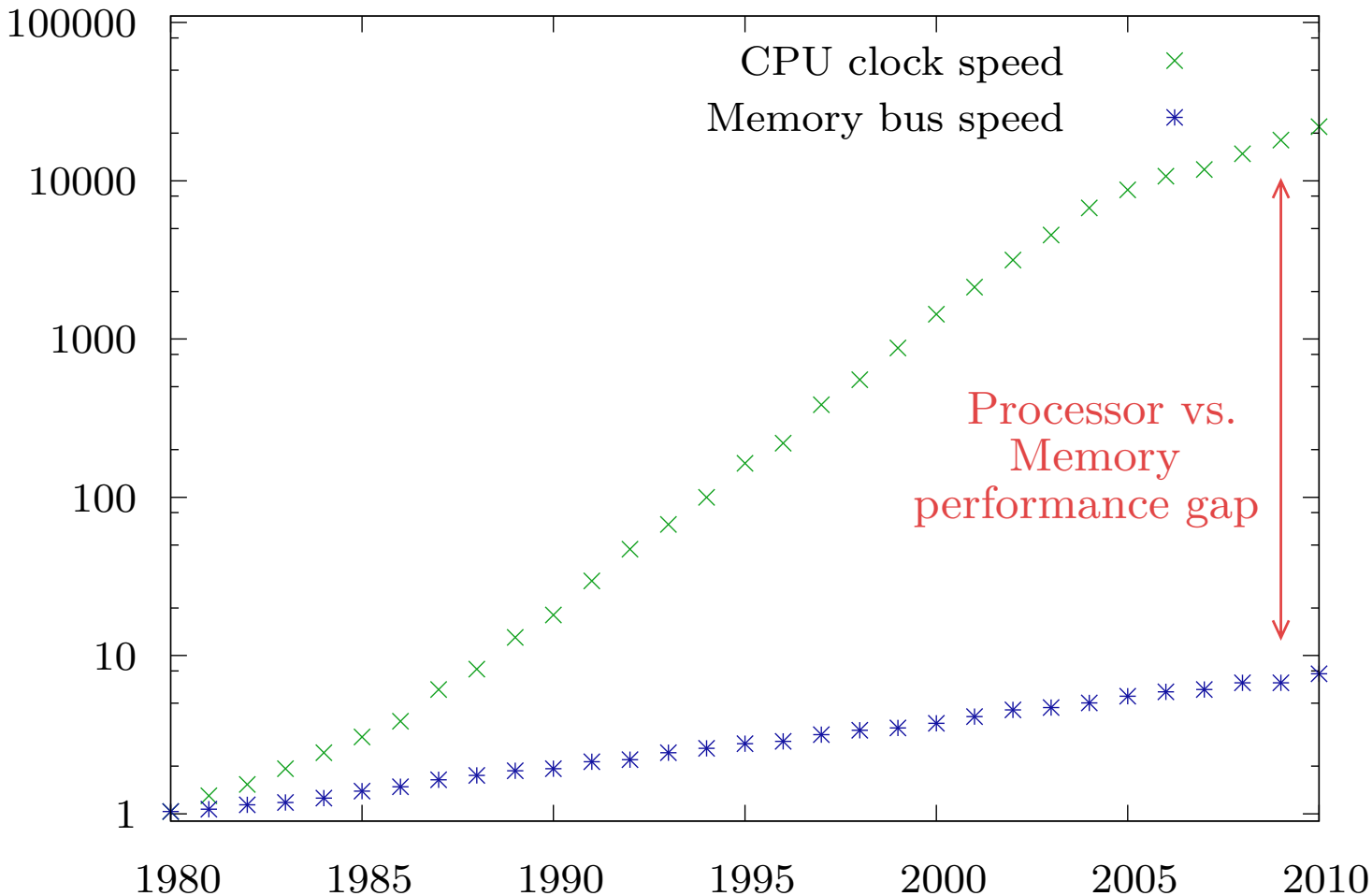

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Lazy matrices

- Stored matrix: All elements reside in memory
- Lazy matrix:
  - Generalisation of matrices
    - State
    - Non-linear
    - Elements may be expressions

  $\Rightarrow$ Obtaining elements expensive

  - Evaluation of internal expression: Delayed until `contraction`
  - For convenience: Offer matrix-like interface

Using lazy matrices

- Program as usual

$$\mathbf{D} = \mathbf{A} + \mathbf{B}$$

- Build expression tree internally

$$\boxed{\mathbf{D}} = \boxed{\mathbf{A}} + \boxed{\mathbf{B}}$$

- On application:

$$\mathbf{D}\underline{x} = (\mathbf{A}\underline{x}) + (\mathbf{B}\underline{x})$$

Using lazy matrices

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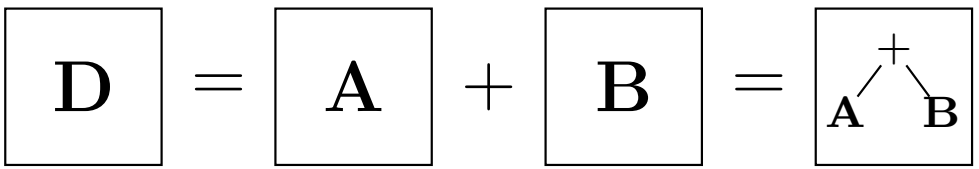

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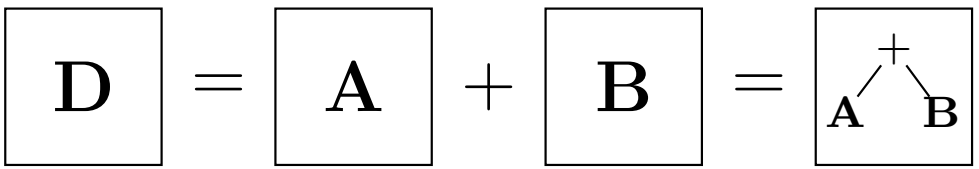


- On application:

$$\mathbf{D}\underline{\boldsymbol{x}} = (\mathbf{A}\underline{\boldsymbol{x}}) + (\mathbf{B}\underline{\boldsymbol{x}})$$

Notes and observations

- `lazyten`: Bookkeeping for `contraction`-functions
- Programmer still sees matrices

$\Rightarrow$ Language for writing `contraction`-based algorithms

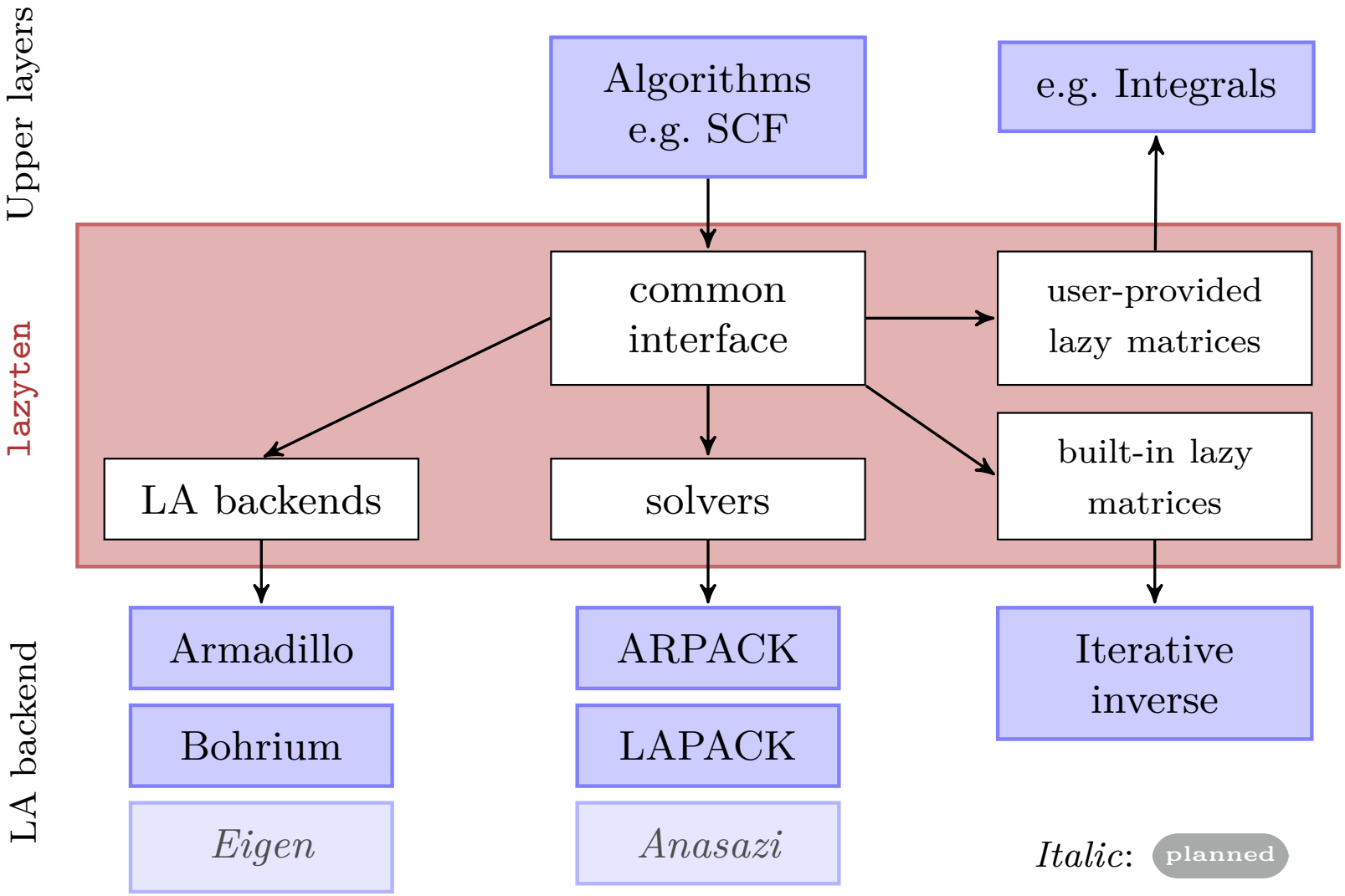
- Lazy matrices allow layered responsibility for computation, e.g. $(\mathbf{A} + \mathbf{B})\underline{\boldsymbol{x}}$
  - $\mathbf{A}\underline{\boldsymbol{x}}$ and $\mathbf{B}\underline{\boldsymbol{x}}$ decided by implementation of $\mathbf{A}$ and $\mathbf{B}$
  - $(\mathbf{A}\underline{\boldsymbol{x}}) + (\mathbf{B}\underline{\boldsymbol{x}})$ done in linear algebra backend

$\Rightarrow$ Proper modularisation between

- Higher-level algorithms
- Lazy matrix implementations
- LA backends

lazyten: Lazy matrix library

Structure of the library



lazyten in practice: Example code

- lazyten[1]: Prototype C++ implementation

```
1  typedef SmallVector<double> vector_type;
2  typedef SmallMatrix<double> matrix_type;
3  auto v = random<vector_type>(100);
4  DiagonalMatrix<matrix_type> diag(v);
5  auto a = random<matrix_type>(100,100);
6  auto b = random<matrix_type>(100,100);
7
8  // No computation: Just build expression tree
9  auto sum = diag + a;
10 auto projector = sum * inverse(sum);
11 auto tree = b - projector * b;
12
13 // Evaluate tree on application:
14 SmallVector<double> res = tree * v;
```

[1] https://lazyten.org

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Lazy matrices for quantum chemistry codes

- `contraction`-based algorithms

⇒ Lower memory footprint, scaling improvements

- Readable code

⇒ Great for teaching or to play around

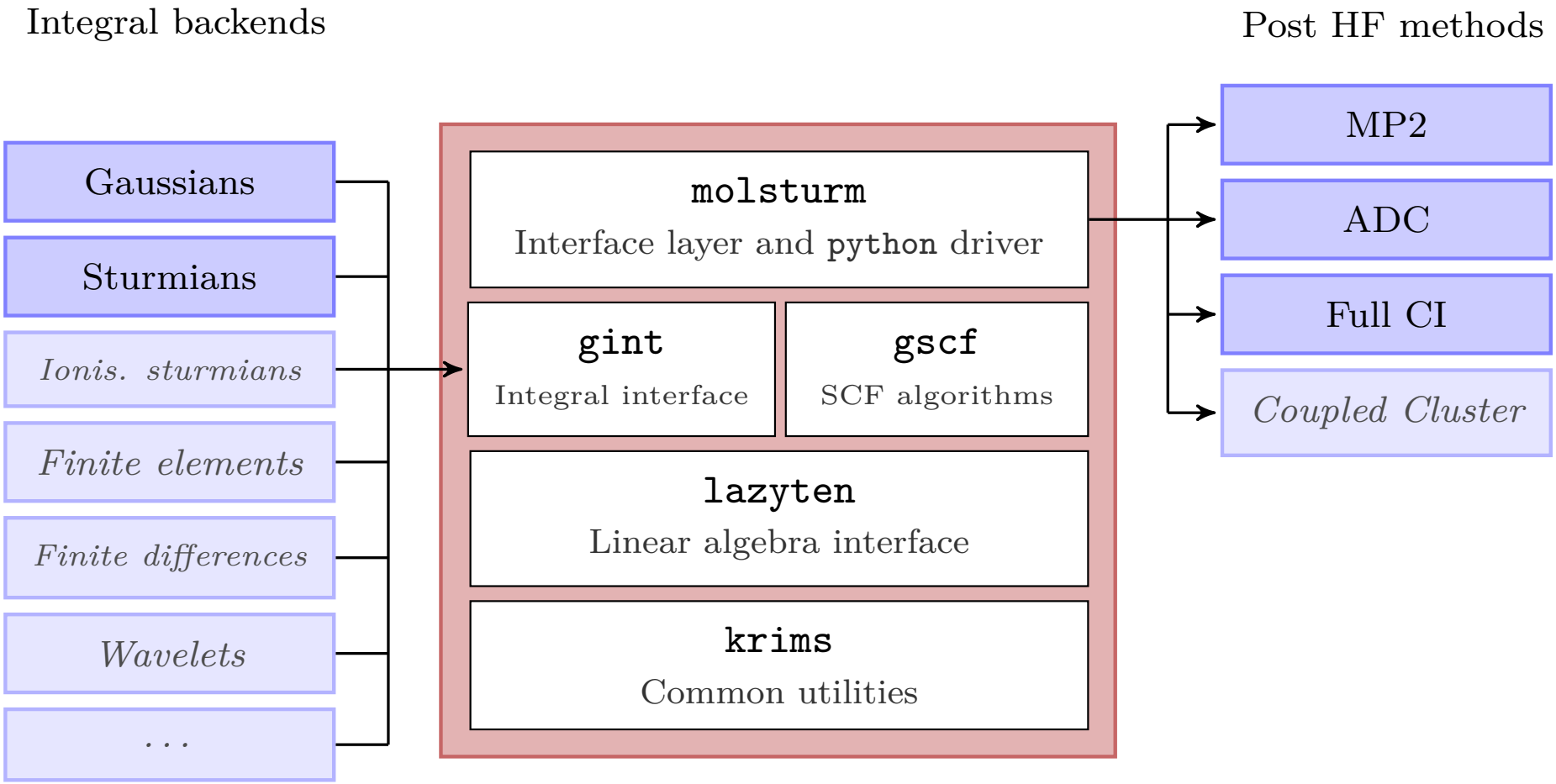
- Abstraction between integrals and SCF algorithms

⇒ Plug and play integral libraries

⇒ Swap LA backends

⇒ Basis-type independent SCF / quantum chemistry

molsturm structure



- *Italic*: planned

molsturm design

- Enables `contraction`-based SCF routines
- Flexiblity as primary goal
- Behaviour controlled via `python`
  - Keywords to change basis type or solver
  - All computed data available in `numpy` format
  - No input file, just a `python` script
- `python` utilities
  - Import / export results
  - Post-HF calculations

molsturm interface: CCD residual (parts)

$$
\begin{aligned}
r_{ij}^{ab} = &- \frac{1}{2} \sum_{mnef} \langle mn||ef\rangle \, t_{mn}^{af} \, t_{ij}^{eb} + \frac{1}{2} \sum_{mnef} \langle mn||ef\rangle \, t_{mn}^{bf} \, t_{ij}^{ea} - \frac{1}{2} \sum_{mnef} \langle mn||ef\rangle \, t_{in}^{ef} \, t_{mj}^{ab} \\
&+ \frac{1}{2} \sum_{mnef} \langle mn||ef\rangle \, t_{jn}^{ef} \, t_{mi}^{ab} + \frac{1}{4} \sum_{mnef} \langle mn||ef\rangle \, t_{mn}^{ab} \, t_{ij}^{ef} + \frac{1}{2} \sum_{mnef} \langle mn||ef\rangle \, t_{im}^{ae} \, t_{jn}^{bf} \\
&- \frac{1}{2} \sum_{mnef} \langle mn||ef\rangle \, t_{jm}^{ae} \, t_{in}^{bf} - \frac{1}{2} \sum_{mnef} \langle mn||ef\rangle \, t_{im}^{be} \, t_{jn}^{af} + \frac{1}{2} \sum_{mnef} \langle mn||ef\rangle \, t_{jm}^{be} \, t_{in}^{af}
\end{aligned}
$$

```
eri_phys = state.eri.transpose((0, 2, 1, 3))
eri = eri_phys - eri_phys.transpose((1, 0, 2, 3))
res = \
    - 0.5  * np.einsum("mnef,manf,iejb->iajb", eri.block("oovv"), t2, t2) \
    + 0.5  * np.einsum("mnef,mbnf,ieja->iajb", eri.block("oovv"), t2, t2) \
    - 0.5  * np.einsum("mnef,ienf,majb->iajb", eri.block("oovv"), t2, t2) \
    + 0.5  * np.einsum("mnef,jenf,maib->iajb", eri.block("oovv"), t2, t2) \
    + 0.25 * np.einsum("mnef,manb,iejf->iajb", eri.block("oovv"), t2, t2) \
    + 0.5  * np.einsum("mnef,iame,jbnf->iajb", eri.block("oovv"), t2, t2) \
    - 0.5  * np.einsum("mnef,jame,ibnf->iajb", eri.block("oovv"), t2, t2) \
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```

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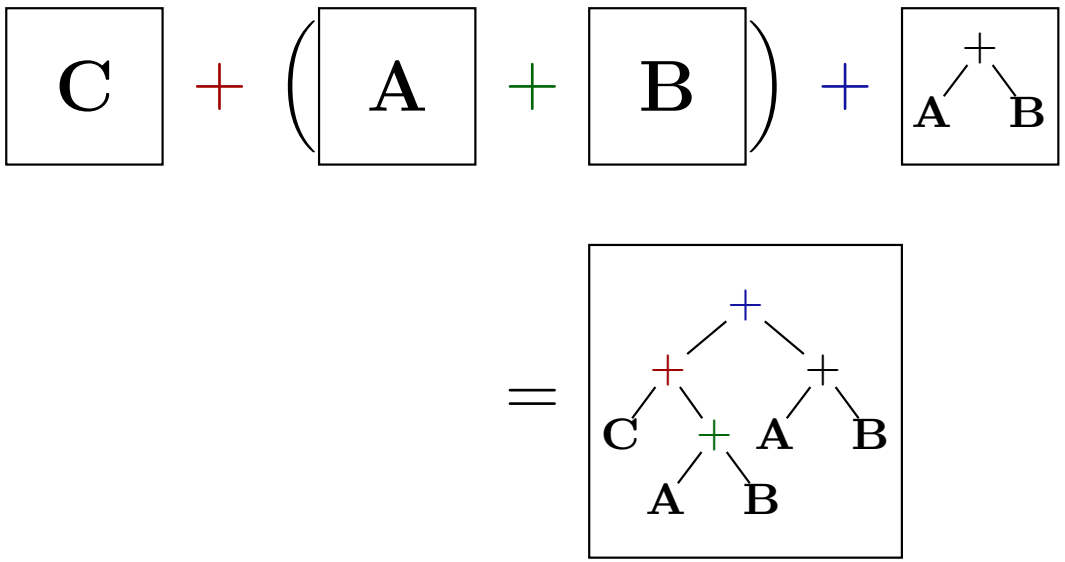
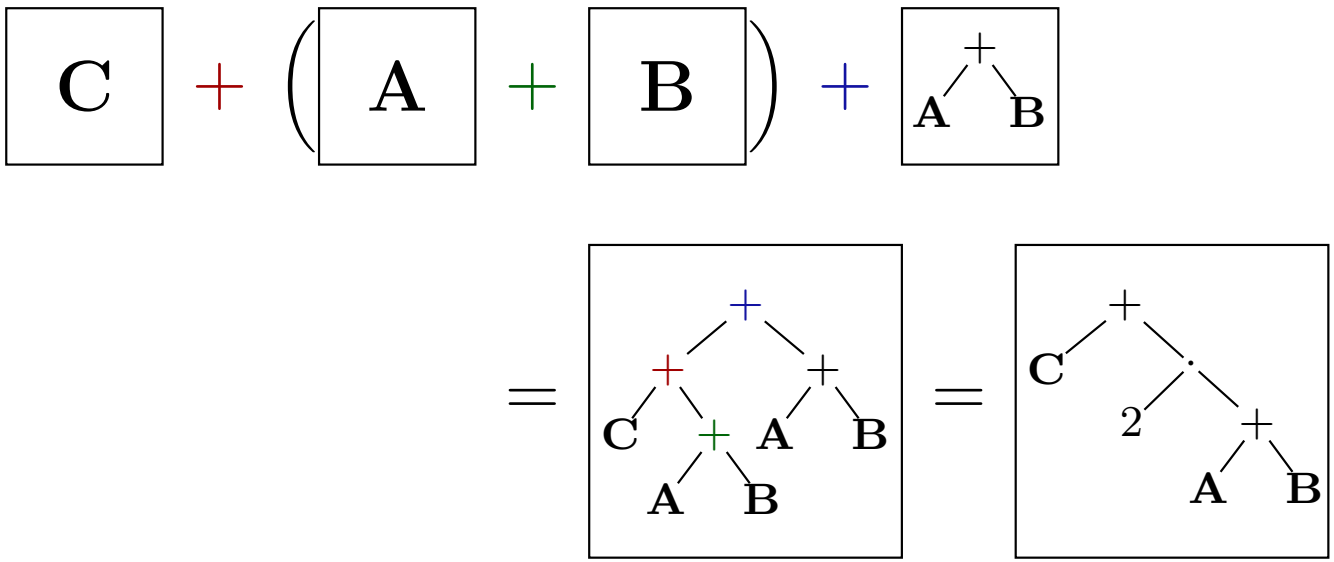
Lazy matrix expression optimisation



- Matrix expression tree ≡ abstract syntax tree ≡ DAG

⇒ May be optimised by standard methods

Lazy matrix expression optimisation



- Matrix expression tree ≡ abstract syntax tree ≡ DAG

⇒ May be optimised by standard methods

Selection of LA backend

- Right now: LA backend is compiled in
- e.g. Bohrium backend
  - Uses just-in-time (JIT) compilation
  - Very specific for hardware
  - Compilation takes time
- Better: Dynamic selection
  - Load on the expression tree
  - Availablility of backends
  - Hardware specs

Extension to lazy tensors

- `contraction` is a special tensor contraction

$\Rightarrow$ Lazy tensors:

- Delay all tensor contractions as long as possible

$$\text{e.g.} \qquad \tilde{k}_{bf} = \sum_{acdo\mu\nu} \mathcal{C}_{ao} \; c^{\mu}_{ab} I_{\mu\nu} c^{\nu}_{cd} \; \mathcal{C}_{co} \mathcal{C}_{df}$$

- Compare possible contraction schemes by complexity
- Execute cheapest evaluation scheme
- May incorporate and exploit symmetry

$\Rightarrow$ Determine optimal contraction sequence automatically

Acknowledgements

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Questions?

- EMail: `michael.herbst@iwr.uni-heidelberg.de`
- Website/blog: `https://michael-herbst.com`
- Projects: `https://lazyten.org` and `https://molsturm.org`