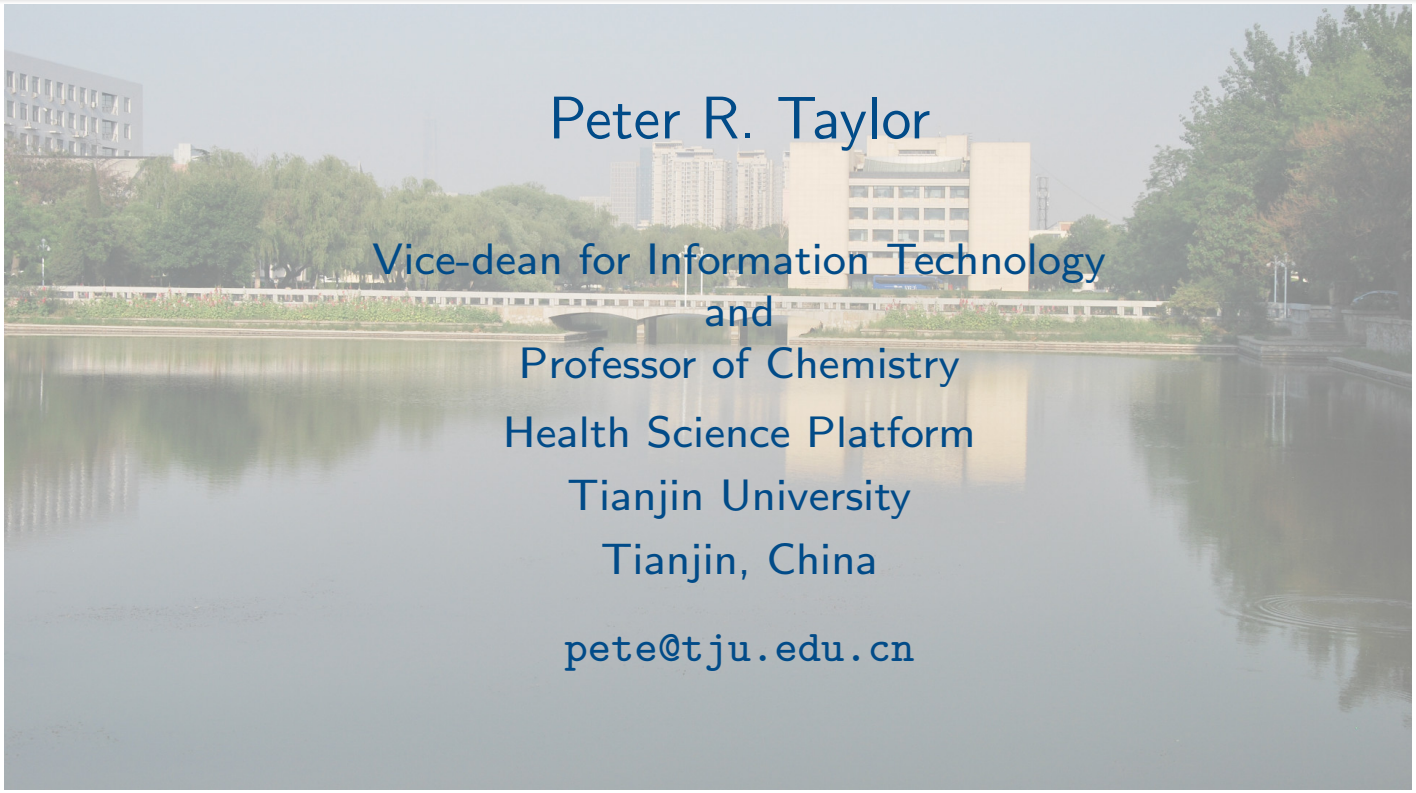
Computational Linear Algebra



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Molecules
Medicine
Biomedical Engineering
Life Science
Public Health Policy
Informatics


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Computational linear algebra

- Some history; processors and vendor roadmaps: current designs, multicore issues, GPUs, TPUs, FPGAs. Caching and virtual memory
- Review of (mostly real) linear algebra: vectors and matrices, determinants, matrix/vector operations (BLAS), block matrix operations.
- Programming: languages, libraries (BLAS, LAPACK, etc.), OpenMP/OpenACC, MPI, CUDA, Scalapack/BLACS.
- Standard methods: matrix multiplication, matrix transformations, Gaussian elimination, matrix diagonalization, singular value decomposition, Cholesky factorization.

Computational linear algebra

- Performance measurement: strategies, code optimization and debugging packages.
- Optimization of functions: first- and second-order methods, constraints, trust-region methods.
- Large systems: linear and nonlinear equations, diagonalization
- Factorization methods (Cholesky, resolution of the identity) in computational chemistry.

Recommended reading

- Golub and van Loan "Matrix Computations" (Johns Hopkins, 4th ed).
- Strang "Linear Algebra and its Applications" (Brooks Cole, 4th ed [or higher now?]).
- Fletcher "Practical Methods of Optimization" (Wiley, 2nd ed).

Ancient history

- 1940s/1950s technology: vacuum tubes, mercury delay lines...
- 1960s: semiconductors — ferrite core memory, tapes (sequential storage).
- 1970s: integrated circuits ("chips"), semiconductor memory, disk/drum storage (random access storage).

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- Seymour Cray and the revolution...

Seymour Cray

- UNIVAC to Control Data: sole interest was *creating the fastest machine around*.
- CDC6600: pathway to CDC7600. Pipelining
- E.g., FP add
  - Load operands into arithmetic unit
  - Unpack reals and shift to match exponents
  - Add
  - Pack to standard FP form
  - Store result
- Old-skool: complete one add, then start next.
- Cray: multi-stage CPU pipeline, *start next operation every clock tick.*

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- Cray left (on good terms) to use his design for his own company.

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- Had to *abandon* old ideas about memory use!
- Had to ensure that all compute-intensive work was implemented as simple vector loops or as matrix operations.

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- Rewriting led to cleaner, simpler code that compilers could more easily optimize, and which usually took more advantage of optimized vendor libraries.
- Many vendors followed: IBM 3090VF, CDC Cyber205, and Cray went on to produce the multiprocessor X–MP, the "huge" memory (2GB in 1985) Cray 2, and follow-ons to both.

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- Much of the functionality was incorporated into mainstream processors (e.g., Intel's AVX) and supported by their libraries.
- Physics is against faster and faster processors: power draw goes as $(\text{frequency})^3$.
- Inevitably, then, processor speed plateaus and the only way to increase performance is to have *and use* more processors: parallel computing...

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- Our task is *multilevel* parallelism: multicore processors and multiple processors. *Fine-* and *coarse-grained* parallelism.

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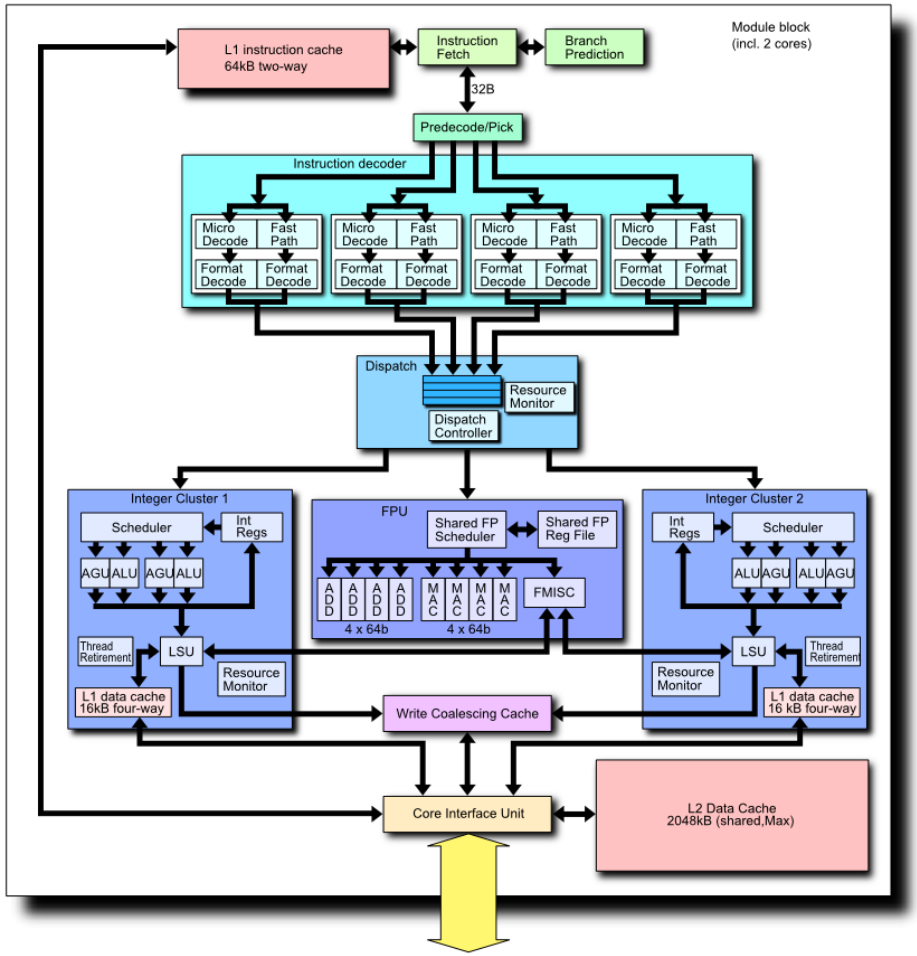
- We have to see...

Typical x86


Module block
(incl. 2 cores)
L1 instruction cache
64kB two-way
Instruction
Fetch
Branch
Prediction
32B
Predecode/Pick
Instruction decoder
Micro
Decode
Fast
Path
Format
Decode
Dispatch
Resource
Monitor
Dispatch
Controller
Integer Cluster 1
Scheduler
Int
Regs
AGU
ALU
Thread
Retirement
LSU
Resource
Monitor
L1 data cache
16kB four-way
FPU
Shared FP
Scheduler
Shared FP
Reg File
ADD
MAC
FMISC
4 x 64b
Integer Cluster 2
Write Coalescing Cache
Core Interface Unit
L2 Data Cache
2048kB (shared,Max)
L1 data cache
16 kB four-way

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- Need lightweight "threads" of execution as tasks: quite different from traditional UNIX/Linux `fork/exec`.
- "Hyperthreading" to maximize use of cores: workload-dependent.

Vectors

- Vector space $\{\mathbf{x}^k\}$

$$\alpha(\mathbf{x}^i + \mathbf{x}^j) = \alpha\mathbf{x}^i + \alpha\mathbf{x}^j.$$

  k-dimensional vector space.
- k need not be finite.
- Linear independence:

$$\sum_i \alpha_i \mathbf{x}^i = 0 \Rightarrow \alpha_i = 0 \,\forall\, i.$$

- Otherwise the set is *linearly dependent*.

Vectors

- Write as columns

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_k \end{pmatrix}$$

  for a k-dimensional vector space.

- *Transpose* is a row vector

$$\mathbf{x}^T = (x_1\ x_2\ \cdots\ x_k)$$

Scalar product

- Two vectors $\mathbf{x}$ and $\mathbf{y}$:

$$\mathbf{x} \cdot \mathbf{y} \equiv \langle \mathbf{x} | \mathbf{y} \rangle = \mathbf{x}^T \mathbf{y} = \sum_p x_p y_p.$$

- $\mathbf{x} \cdot \mathbf{x} \geq 0$.
- *Orthonormal* vector space:

$$\mathbf{x}^i \cdot \mathbf{x}^j = \delta_{ij}.$$

Matrices

- Array of elements

$$\mathbf{A} = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mn} \end{pmatrix}.$$

  m rows, n columns. $m \times n$ matrix.
- "Square matrix" if $m = n$.
- *Symmetric* if square and all $A_{pq} = A_{qp}$.

Matrix properties

- Consider as a set of n m-dimensional column vectors, or m n-dimensional row vectors.
- *Span*, *rank*, *kernel*.
- Matrix multiplication **AB**:

$$C_{pq} = \sum_r A_{pr} B_{rq},$$

  matrices must be *compliant*: **A** $m \times k$, **B** $k \times n$, so **C** $m \times n$.
- Holds also for vectors: scalar and *matrix* product.

Norms

- *Vector p-norms*

$$\|x\|_p = \left(\sum_k x_k^p \right)^{\frac{1}{p}}.$$

- $\|x\|_2 = \mathbf{x}^T \mathbf{x}$.
- $\|x\|_\infty = \max |x_i|$.
- *Cauchy-Schwarz* inequality

$$|\mathbf{x}^T \mathbf{y}| \leq \|x\|_2 \, \|y\|_2.$$

Special case of Hölder's inequality.

Norms

- *Matrix p-norms* can be defined analogous to vector p-norms, e.g.,

$$\|\mathbf{A}\|_\infty = \max |A_{ij}|.$$

- *Frobenius norm*

$$\|\mathbf{A}\|_F = \left(\sum_i \sum_j |A_{ij}|^2 \right)^{\frac{1}{2}}$$

Determinants

- Many definitions, e.g.,

$$\det(\mathbf{A}) \equiv |\mathbf{A}| = \sum_{j=1}^{n} (-1)^(j+1) A_{1j} \det(\mathbf{A}_{1j}),$$

  recursively for an $n \times n$ matrix $\mathbf{A}$.
- This is "expanding along the top row".
- $\det(\mathbf{A}_{1j})$ is a *minor* of $\mathbf{A}$, and $(-1)^(j+1) \det(\mathbf{A}_{1j})$ is *cofactor*, or signed minor.
- Key property: if $\det(\mathbf{A}) = 0$, the matrix $\mathbf{A}$ is *singular*: it has no inverse.

Determinants

- "Proper formula", attributed to Leibniz

$$\det(\mathbf{A}) = \sum_P \sigma_P \prod_i A_{iP(i)} \equiv \sum_P \sigma_P \prod_i A_{P(i)i},$$

where P runs over all permutations of the integers $1 \ldots n$, and σ_P is the *sign*, or *parity* of the permutation, according to whether it comprises an odd or even number of transpositions.

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  where P runs over all permutations of the integers $1 \ldots n$, and σ_P is the *sign*, or *parity* of the permutation, according to whether it comprises an odd or even number of transpositions.
- For anyone with a background in group theory, this is a projection operator for the *alternating*, or *antisymmetric* irreducible representation.
- Leads to other related quantities — consider costs for evaluation.

Block operations

- Recursive generalization of matrix operations. E.g., matrices **A** and **B** which have a block structure

$$\mathbf{A} = \left(\begin{array}{ccc|ccc} A_{11} & \cdots & A_{1l} & A_{1(l+1)} & \cdots & A_{1n} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ A_{k1} & \cdots & A_{kl} & A_{k(l+1)} & \cdots & A_{kn} \\ \hline A_{(k+1)1} & \cdots & A_{(k+1)l} & A_{(k+1)(l+1)} & \cdots & A_{(k+1)n} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ A_{m1} & \cdots & A_{ml} & A_{m(l+1)} & \cdots & A_{mn} \end{array}\right),$$

where for same-sized square blocks (not necessary) $2k = m$ and $2l = n$.

Block operations

- Write this as

$$\mathbf{A} = \begin{pmatrix} \mathbf{A}^{11} & \mathbf{A}^{12} \\ \mathbf{A}^{21} & \mathbf{A}^{22} \end{pmatrix}.$$

- Then e.g., $\mathbf{C} = \mathbf{AB}$ becomes

$$\mathbf{C} = \begin{pmatrix} \mathbf{A}^{11}\mathbf{B}^{11} + \mathbf{A}^{12}\mathbf{B}^{21} & \mathbf{A}^{11}\mathbf{B}^{12} + \mathbf{A}^{12}\mathbf{B}^{22} \\ \mathbf{A}^{21}\mathbf{B}^{11} + \mathbf{A}^{22}\mathbf{B}^{21} & \mathbf{A}^{21}\mathbf{B}^{12} + \mathbf{A}^{22}\mathbf{B}^{22} \end{pmatrix}.$$

- This blocking can be any number, not just 2×2. Very valuable in computer implementations (often hidden from users).

Vector and matrix operations

- The BLAS: Basic Linear Algebra Subprograms.
- Fortran source, but often optimized in vendor libraries.
- BLAS1: vector operations that go as n. Dot product, multiplication by a scalar, addition...
- BLAS2: matrix/vector operations that go as n^2, like matrix/vector multiplication, or matrix addition.
- BLAS3: matrix/matrix operations that go as n^3, like matrix multiplication.
- *Kernels* to build more complicated linear algebra operations.

Keep in mind...

- Floating-point (FP) arithmetic is *finite-precision*.
- Read the IEEE standards if you're interested...
- Note that for 64-bit floating point the processor is required to work in at least 128 bits, and return initially and 80-bit result (all transparent to the user).

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- FP arithmetic is not associative! This can impact exploiting parallelism — don't get exactly the same results.

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- And that you know what to do with the result in register 6. . .

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- Interpreted languages: preeminently Python. Easy and good for prototyping.

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- In general, don't reinvent, exploit!

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- Hyperthreading requires care.