A Comparison of Eigensolvers for Large-Scale Three-Dimensional Problems

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- **Funded by US Department of Energy**
- **Located Albuquerque (NM) & Livermore (CA)**
- **8,300 people**
- **Budget: $2 billion per year**
- **Mission of stockpile stewardship**
- **Capabilities:**
  - Biosciences
  - Chemical and Earth sciences
  - Electronics
  - Computer information
  - Nanotechnology
  - …

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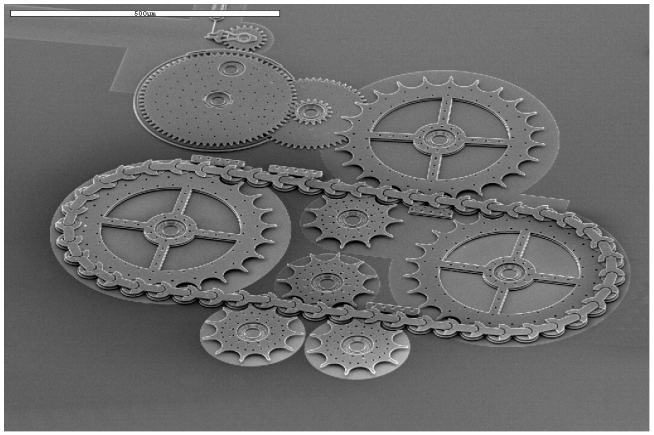
Achievements

Z machine:

- **Achieved an output of 80 times the entire world's output of electricity.**

MEMS:

World's smallest microchain drive



Asci Red:

- **First Tflop system (1.8 Tflops)**
- **9,152 Pentium Pro processors**
- **128 MB per processor**

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Computer Science & Mathematics

- **Development of advanced computing architecture, network, and facilities**
  - ASCI Red: Teraflop system.
  - Cplant: Commodity-based large-scale computing.
- **Software frameworks and solutions for high-performance distributed computing**
  - Trilinos: A collection of solver components.
  - Zoltan: Data management services for parallel applications.
- **Computational methods and codes for selected science and engineering simulations**
  - Dakota: A multilevel parallel, object-oriented framework for design optimization, parameter estimation, uncertainty quantification, and sensitivity analysis.
  - ALEGRA: A three-dimensional, multi-material, arbitrary-lagrangian-eulerian code for solid dynamics.
  - MPSALSA: Massively parallel numerical methods for advanced simulation of chemically reacting flows.
- **Web page: http://www.cs.sandia.gov/**

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CSRI
Computer Science Research Institute

Research in computer science, computational science and mathematics through collaboration with university faculty, students and Sandia staff.

Impact

Research addressing Sandia problems in modeling and simulation
Recruiting through student programs
Improved quality and integration of Sandia research
Increased impact of Sandia research and codes.

Opportunities

Sabbaticals and summer faculty positions,
Postdocs and summer student positions,
Graduate fellowships,
Sponsored workshops, and
Technical visits and colloquia

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Contact: David E. Womble, dewombl@sandia.gov

- **Trilinos is an evolving framework which:**
  - efficiently reuses existing solver technology,
  - leverages new development across various projects,
  - satisfies specified practices for quality assurance.
- **Trilinos is a collection of *packages.***
- **Each package is:**
  - implemented in an object-oriented software framework.
  - focused on important and state-of-the-art algorithms in its problem regime.
  - developed by a small team of domain experts.
  - minimally dependent of parallel machine details.
  - minimally dependent on any other software packages (self-contained).
  - configurable / buildable / documented on its own (portability).
- **Open source: http://software.sandia.gov/trilinos**

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Primary Trilinos Packages

8/4/2003 - v12

- **Basic Linear Algebra Libraries**
  - Epetra: Current Production C++ Library
    - Epetra Core
    - Epetra Extensions
  - Tpetra: Next Generation C++ Library
  - Jpetra: Java Library
- **Common Services**
  - Teuchos: Parameter Lists, BLAS Interfaces, etc
- **Abstract Interfaces and Adaptors**
  - TSFCore: Basic Abstract classes
  - TSF Extensions: Aggregate/composite, overloaded operators
  - TSF Utilities: Core utility classes
- **Linear Solvers**
  - Amesos: OO Interfaces to 3rd party direct solvers
    - SuperLU
    - KundertSparse
    - SuperLUDist
    - DSCPack
    - UMFPack
    - MUMPS
  - AztecOO: Preconditioned Krylov Package based on Aztec
  - Komplex: Complex solver via equivalent real formulations
  - Belos: Next generation Krylov and block Krylov solvers
- **Preconditioners**
  - ML: Multi-level preconditioners
  - Meros: Segregated/Block Preconditioners
  - IFPACK: Algebraic preconditioners
- **Nonlinear Solvers**
  - NOX: Collection of nonlinear solvers
  - LOCA: Library of Continuation Algorithms
- **Eigensolvers**
  - Anasazi: Collection of eigensolvers
- **Time Integration**
  - TOX: Planned development
- **"New Package"**
  - "Hello World": Package Template to aid integration of new packages
  - Web site with layout and instructions

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Trilinos Packages

- **Epetra**
  - Concrete linear algebra classes (matrices, multivectors, graphs, operators, …).
  - Parallel code for linear algebra computations.
  - Portable interface to BLAS and LAPACK.
- **ML**
  - Multilevel preconditioning.
  - Geometric and algebraic multigrid.
- **AztecOO**
  - Based on Aztec.
    - Aztec is extracted from MPSalsa reacting flow code.
  - Algorithms: BiCGSTAB, CG, CGS, GMRES, TFQMR.
- **Anasazi**
  - Collection of eigensolvers

Problem

$$KQ = MQ\Lambda$$

- **K is a sparse and symmetric matrix *(stiffness).***
- **M is a sparse, symmetric, positive, definite matrix *(mass)*.**

  - **Frequency response in structural dynamics**
  - **Cavity analisys in electromagnetism**
  - **…**

Objective:

Determine the next generation approach to solve a generalized eigenproblem for extremely large 3D problems high into the frequency range

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Overview of Methods

- **Lanczos Method**
  - Boeing code — R. Grimes, J. Lewis, and H. Simon (1994)
  - Salinas code — 2002 Gordon Bell Prize Winner
- **Preconditioned Eigensolver**
  - The linear system $\mathbf{Ku} = \mathbf{f}$ is not solved accurately.
- **Component Mode Synthesis**
  - Over the last year, the AMLS method has become dominant for the frequency response analysis in the car industry.

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Lanczos Method

$$(K-\sigma M)^{-1}MV = VT + \sigma u e^{T}$$

- $V^{T}MV = I$.
- T is a tridiagonal matrix.
- Implicitly restarted Lanczos method (ARPACK).

Key computational issue: $x \rightarrow (K-\sigma M)^{-1}x$

- Boeing Code: Sparse factorization
- Salinas Code: Scalable FETI-DP solver (Farhat)

$$\sigma \leq 0$$

- Experiments: PCG with AMG preconditioner

$$\sigma = 0$$

Reference: R. Lehoucq, D. Sorensen, and C. Yang (1998)

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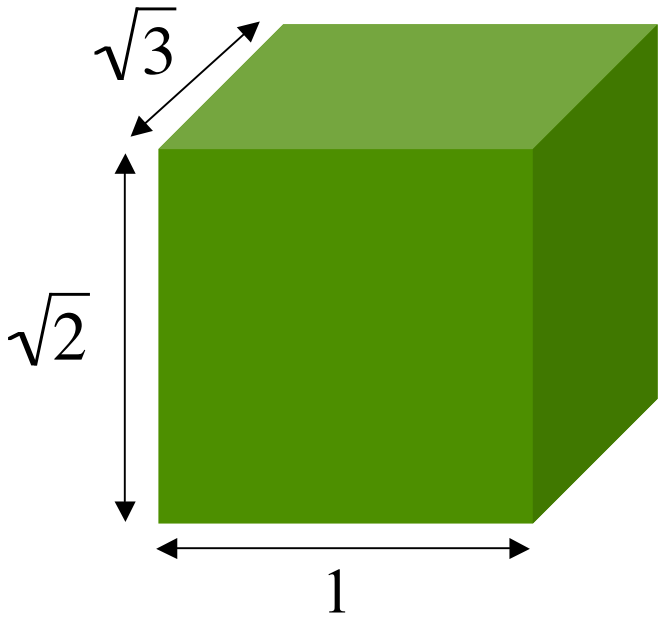
Model Problem



- We consider the Laplace equation with Dirichlet condition.
- The continuous eigenvalues can be multiple.
- The unit cube is discretized with 101 Q1 elements per direction.
- The smallest discrete eigenvalues are simple.

Platform and other details

- 16 processors (Dec Alpha processors).
- 512 MB memory per processor.
- CXML LAPACK and BLAS.
- All codes but ARPACK are in C++.
- The mass and stiffness matrix-vector multiplications are blocked (Epetra framework).
- The AMG preconditioner does not operate per block.

Post-processing checks:

- Mass-orthonormality of eigenvectors
- Missed eigenpairs
- Angles between the computed and discrete eigenspaces

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Convergence Check

Theoretical result:

$$|\lambda - \lambda_0| \leq \frac{\|Kx - Mx\lambda\|_{M^{-1}}}{\|x\|_M}$$

Convergence criterion:

$$\frac{1}{\sqrt{\lambda_1}} \frac{\|Kx - Mx\lambda\|_2}{\|x\|_M} \leq \varepsilon$$

- λ_1 is the smallest eigenvalue of M
- ε is the tolerance ($10^{-4} \approx$ discretization error)

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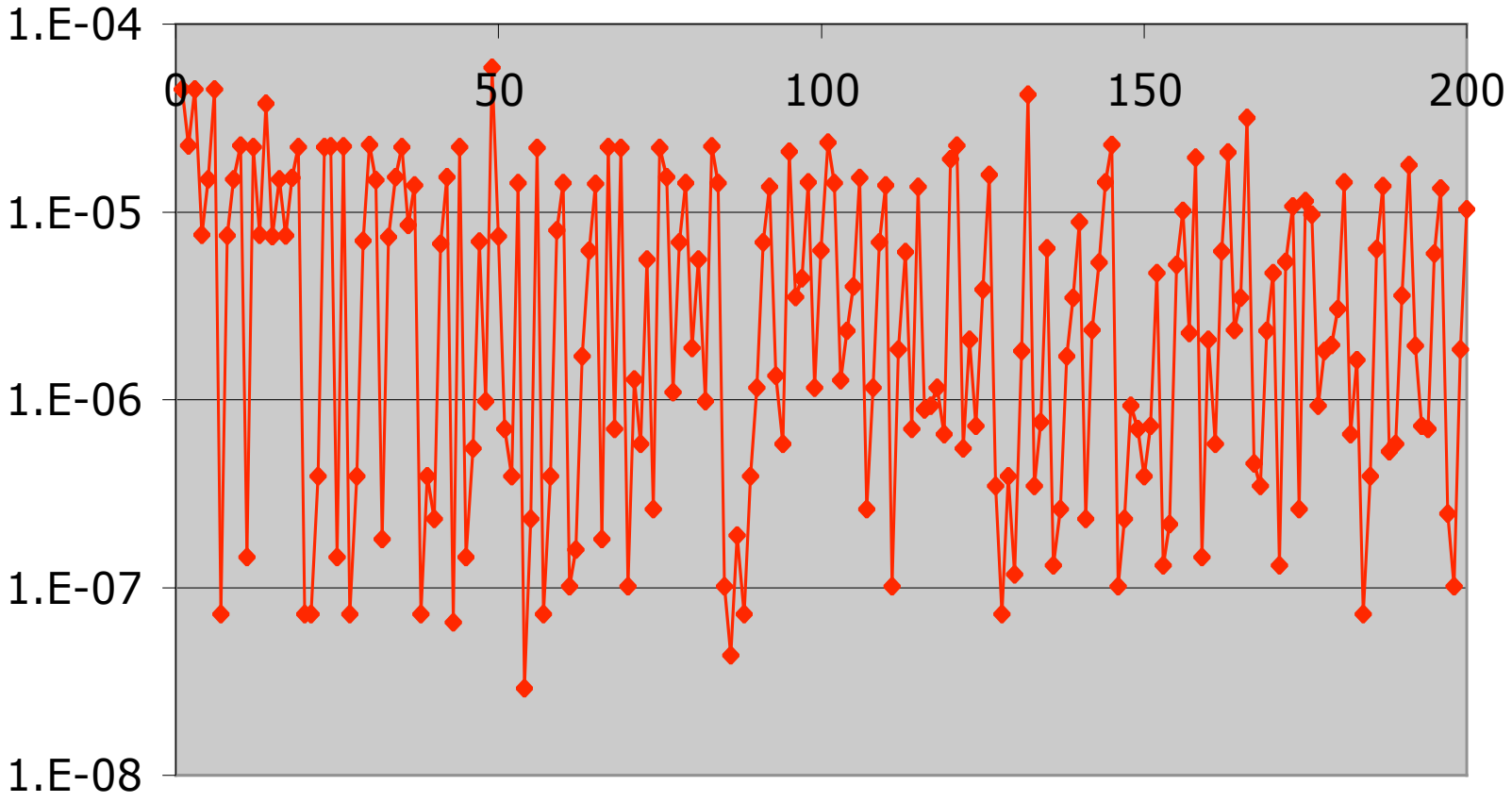
Gap

$$\text{Gap} = \frac{\lambda_{j+1} - \lambda_j}{\lambda_{max} - \lambda_{min}}$$

Spread ≈ $2*10^5$



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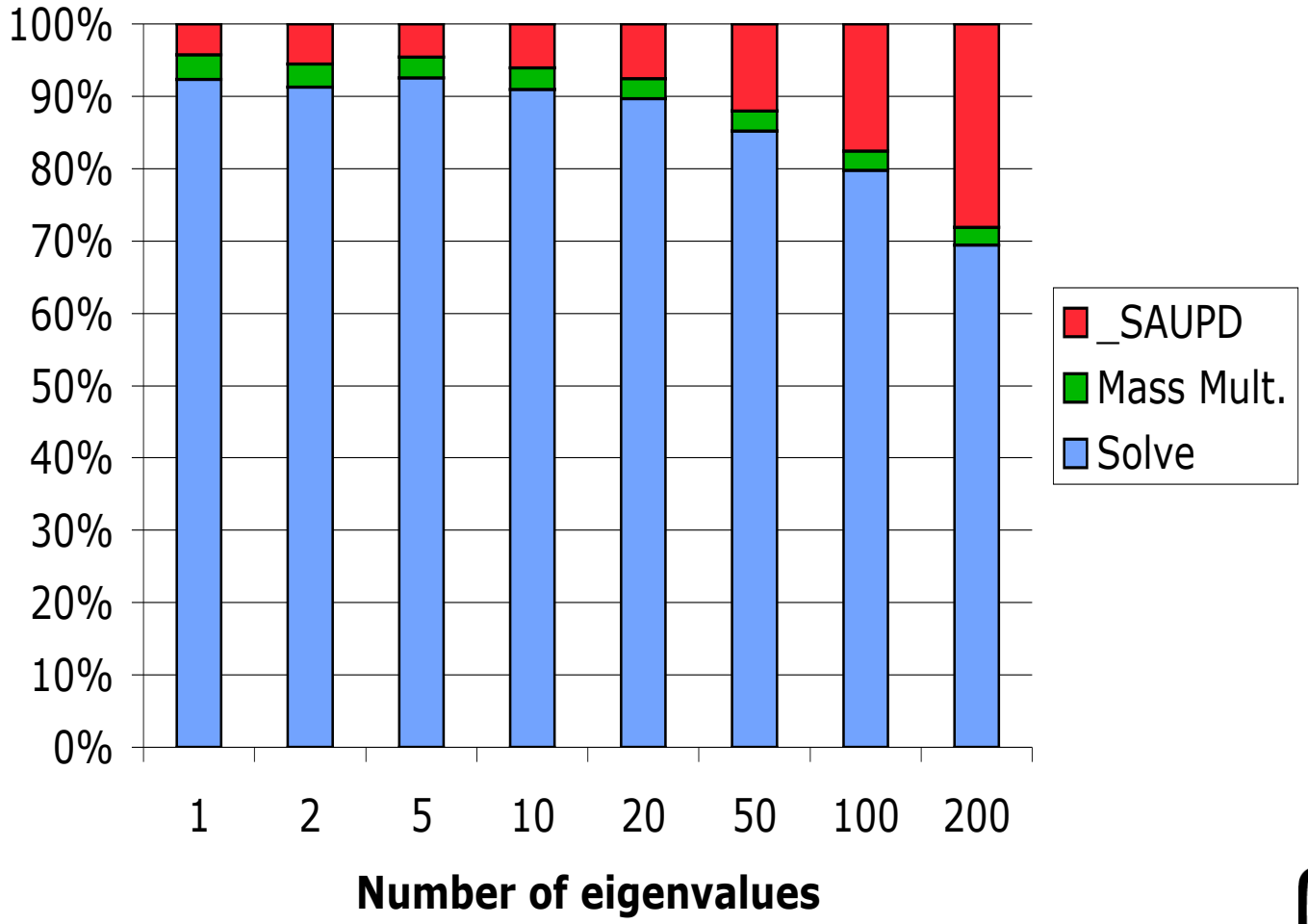
Time Distribution for ARPACK

- Number of eigenvalues requested: nev
- Size of working space: 2*nev



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Preconditioned Eigensolver

Idea: **Replace the operation $x \rightarrow (K-\sigma M)^{-1}x$ by $x \rightarrow N^{-1}x$ where N is a preconditioner for $K-\sigma M$**

Algorithms:

- **Gradient-based schemes: DACG & LOBPCG**
  - Minimization of Rayleigh quotient
  - Fixed subspace size
  - Conjugate gradient algorithm
- **Newton-based schemes:**
  - Block Davidson
  - Block Jacobi-Davidson

Important note: **We use a preconditioner N for K ($\sigma = 0$).**

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Block DACG

- The algorithm minimizes the Rayleigh quotient on the space

$$\mathrm{Span}\{X^{(i)}, P^{(i)}\}$$

- The search directions $P^{(i)}$ are defined by

$$P^{(i)} = -N^{-1}(KX^{(i)} - MX^{(i)}\Lambda^{(i)}) + P^{(i-1)}B^{(i)}$$

- The matrix $B^{(i)}$ uses the Bradbury-Fletcher formula

$$B^{(i)} = \frac{\mathrm{diag}\left[\left(KX^{(i)} - MX^{(i)}\Lambda^{(i)}\right)^{T} N^{-1}\left(KX^{(i)} - MX^{(i)}\Lambda^{(i)}\right)\right]}{\mathrm{diag}\left[\left(KX^{(i-1)} - MX^{(i-1)}\Lambda^{(i-1)}\right)^{T} N^{-1}\left(KX^{(i-1)} - MX^{(i-1)}\Lambda^{(i-1)}\right)\right]}$$

- The classical Gram-Schmidt algorithm is used for orthogonalization.
- The eigenvectors are deflated at convergence.

Reference: L. Bergamaschi and M. Putti (2002)

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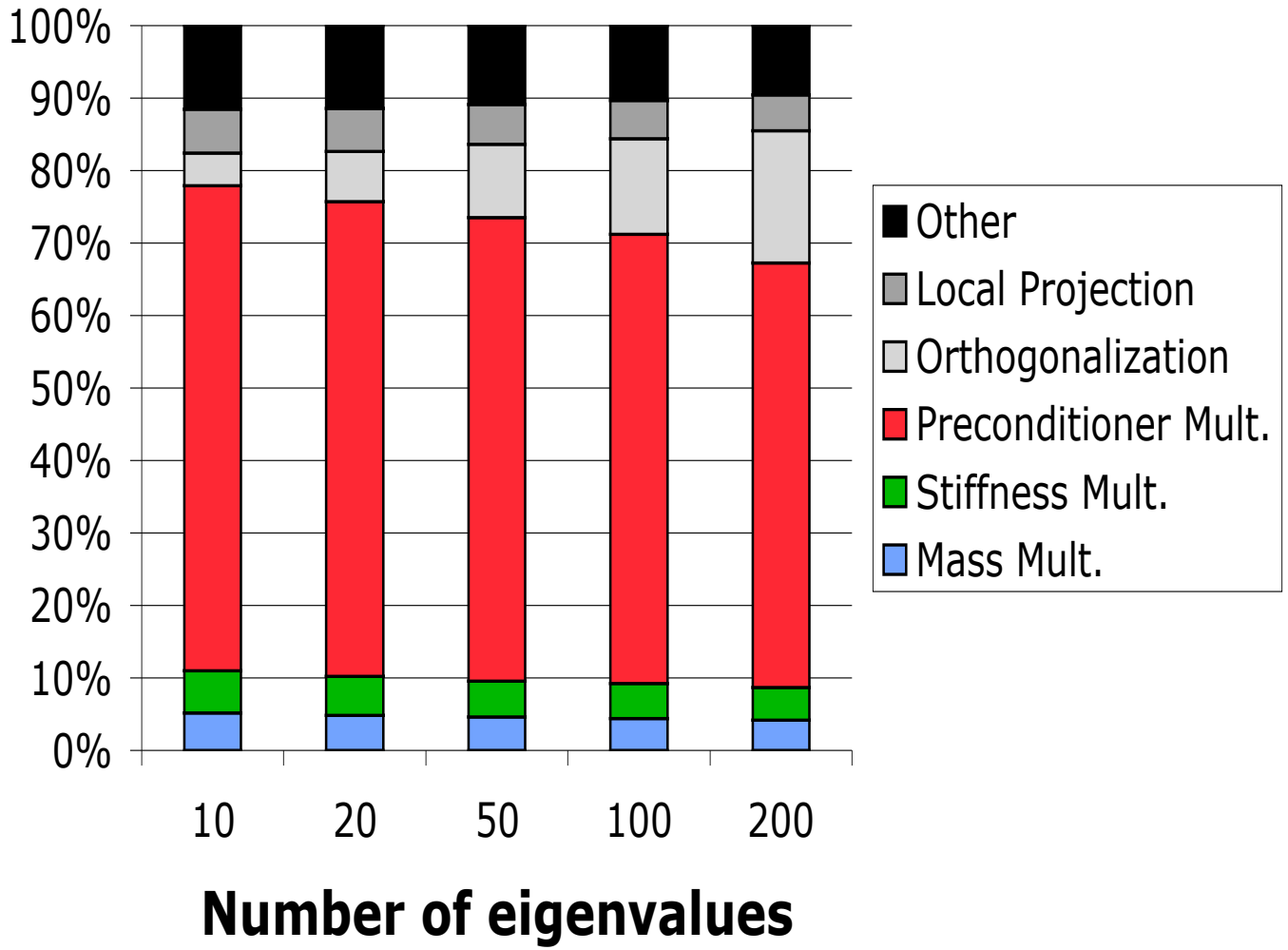
Time Distribution for DACG (10)



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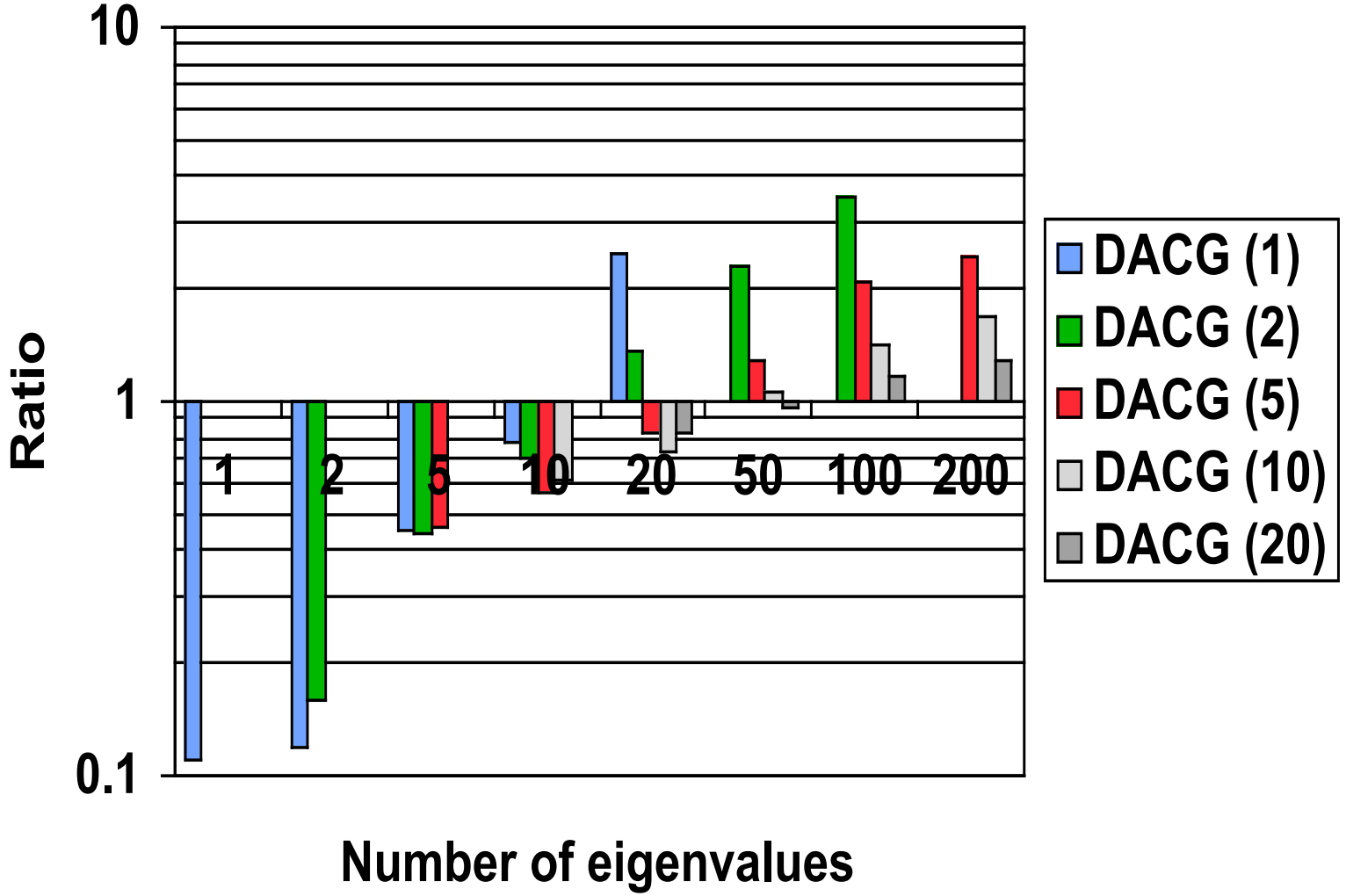
Relative Time vs ARPACK



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LOBPCG

- The incremental idea is to use a three-term recurrence à la Lanczos.
- The algorithm minimizes the Rayleigh quotient on the space

$$\mathrm{Span}\{X^{(i)}, X^{(i-1)}, N^{-1}(KX^{(i)}-MX^{(i)}\Lambda^{(i)})\}$$

- The classical Gram-Schmidt algorithm is used for orthogonalization.
- The eigenvectors are deflated at convergence.

Reference: A. Knyazev (2001)

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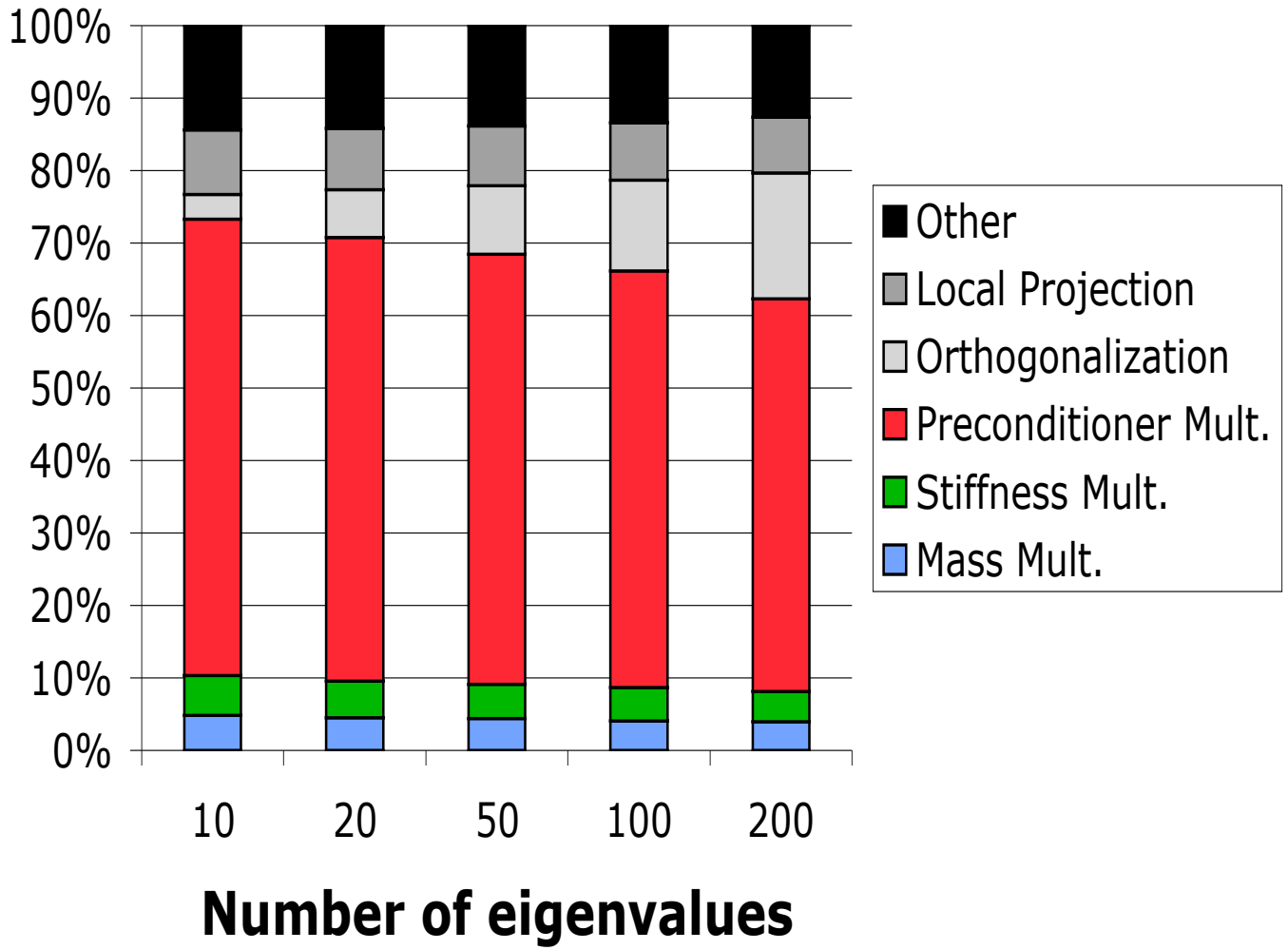
Time Distribution for LOBPCG (10)



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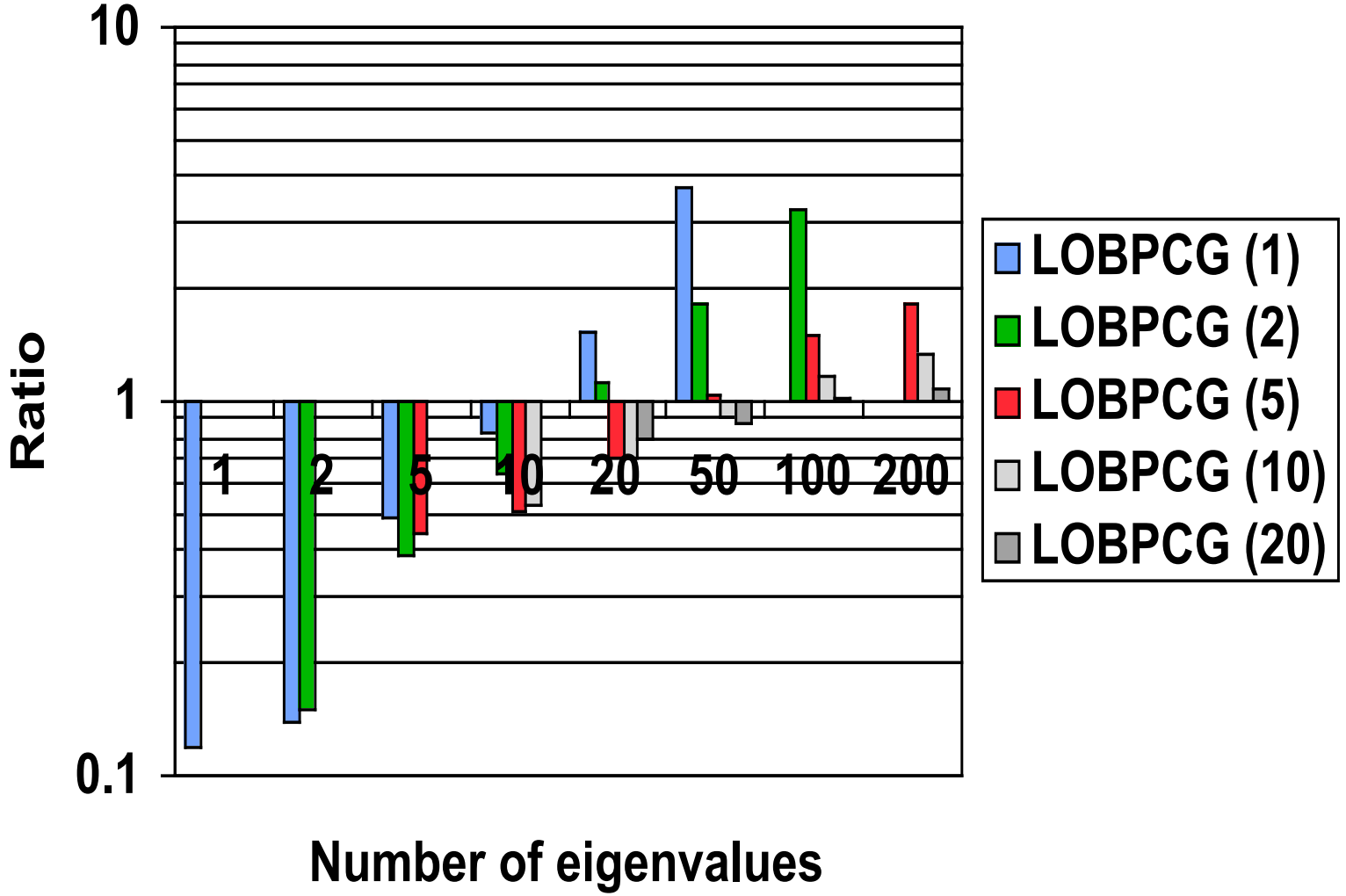
Relative Time vs ARPACK



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Davidson Algorithm

- The algorithm minimizes the Rayleigh quotient on the space

$$\text{Span}\{X^{(0)},\ N^{-1}(KX^{(0)}-MX^{(0)}\Lambda^{(0)}),\ \ldots$$

$$N^{-1}(KX^{(m-1)}-MX^{(m-1)}\Lambda^{(m-1)}),\ N^{-1}(KX^{(m)}-MX^{(m)}\Lambda^{(m)})\}$$

- For nev eigenvalues requested, the subspace is restarted when the size reaches 2*nev.
- The preconditioner N is fixed for all the computation.
- An M-orthonormal basis is generated for the subspace.
- The eigenvectors are deflated at convergence.

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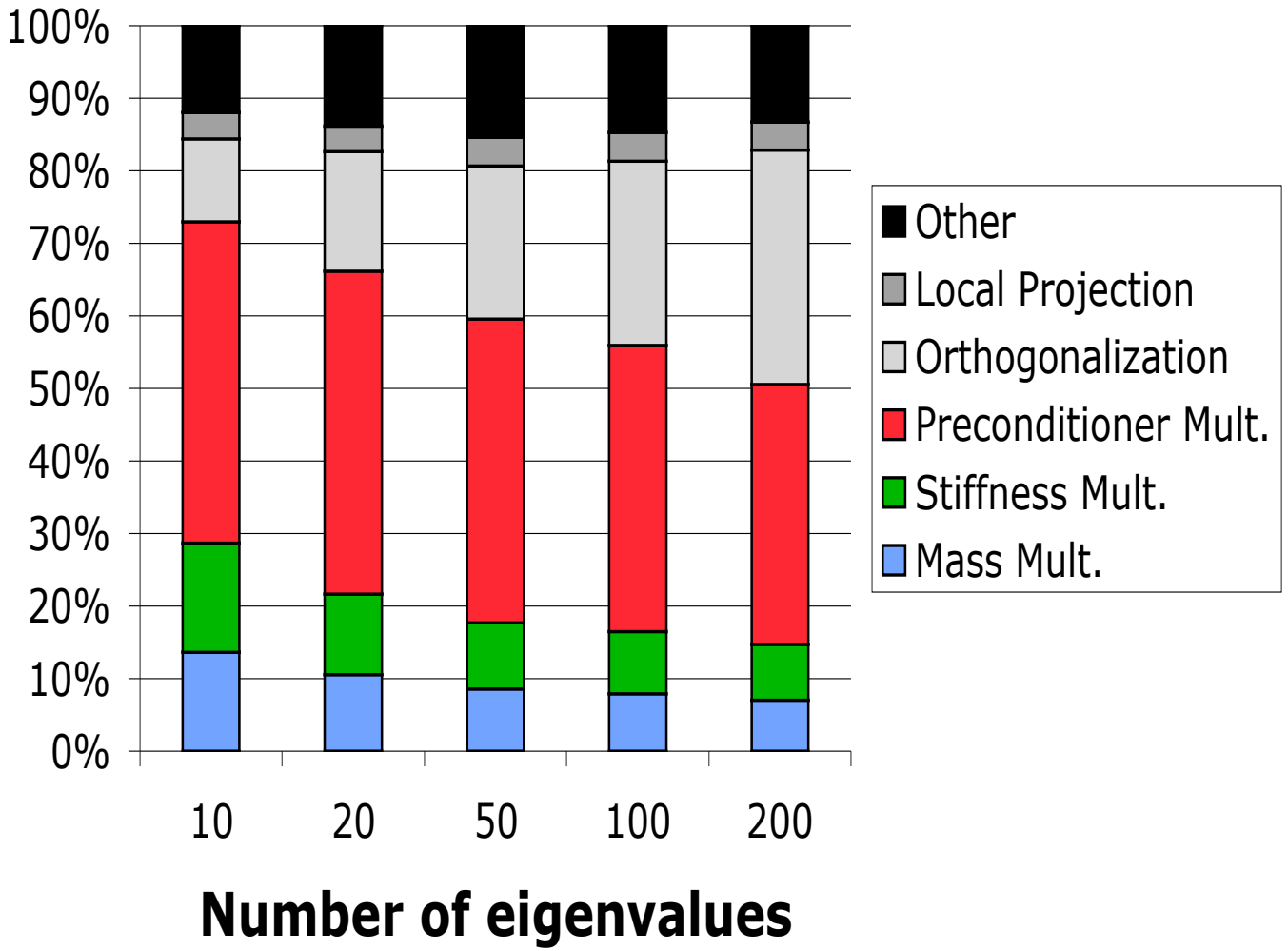
Time Distribution for Davidson (10)



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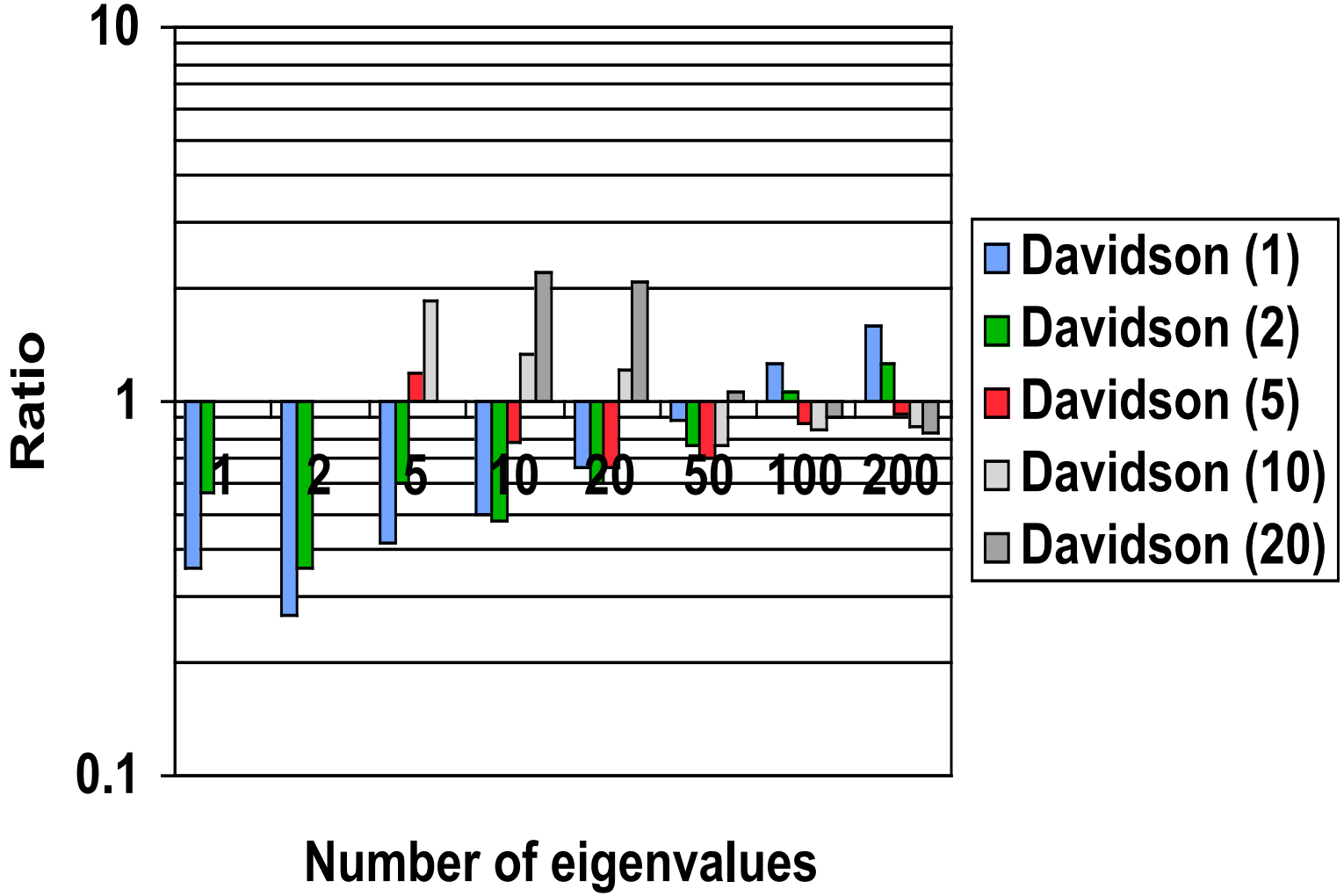
Relative Time vs ARPACK



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Jacobi Davidson

- The algorithm is based on the Davidson algorithm.
- The correction equation improves the computed eigenvector

$$(I-MQQ^T)(K-\lambda M)(I-QQ^TM)Z = -(I-MQQ^T)(KX-MX\Lambda)$$

- The correction equation is solved with preconditioned conjugate gradient

$$(I-MQQ^T)N(I-QQ^TM)$$

- The preconditioner N is fixed for all the computation.
- An M-orthonormal basis is generated for the subspace.
- The eigenvectors are deflated at convergence.

Reference: G. Sleijpen and H. Van Der Vorst (1996), Y. Notay (2001)

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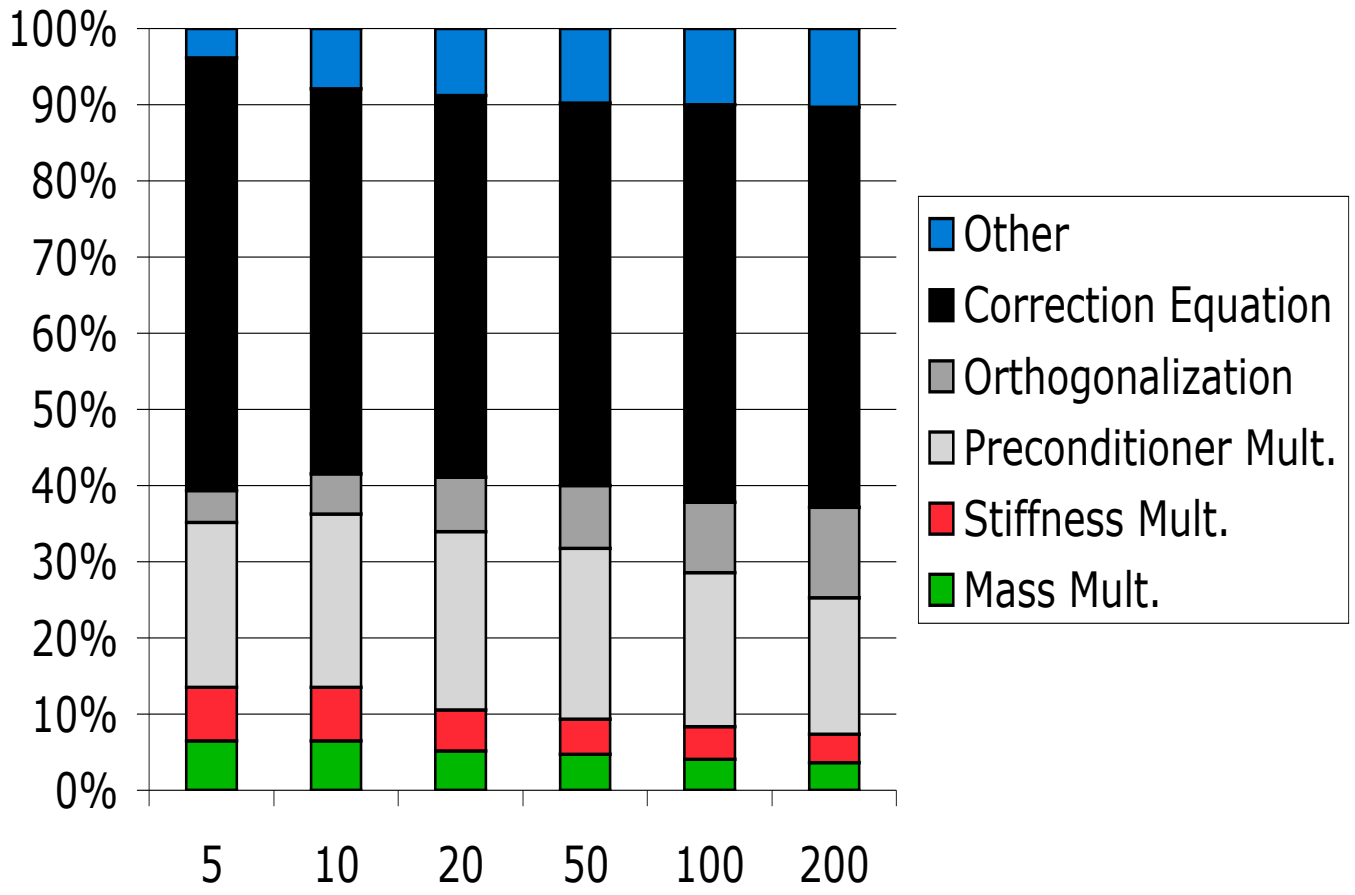
Time Distribution for JDPCG (5)



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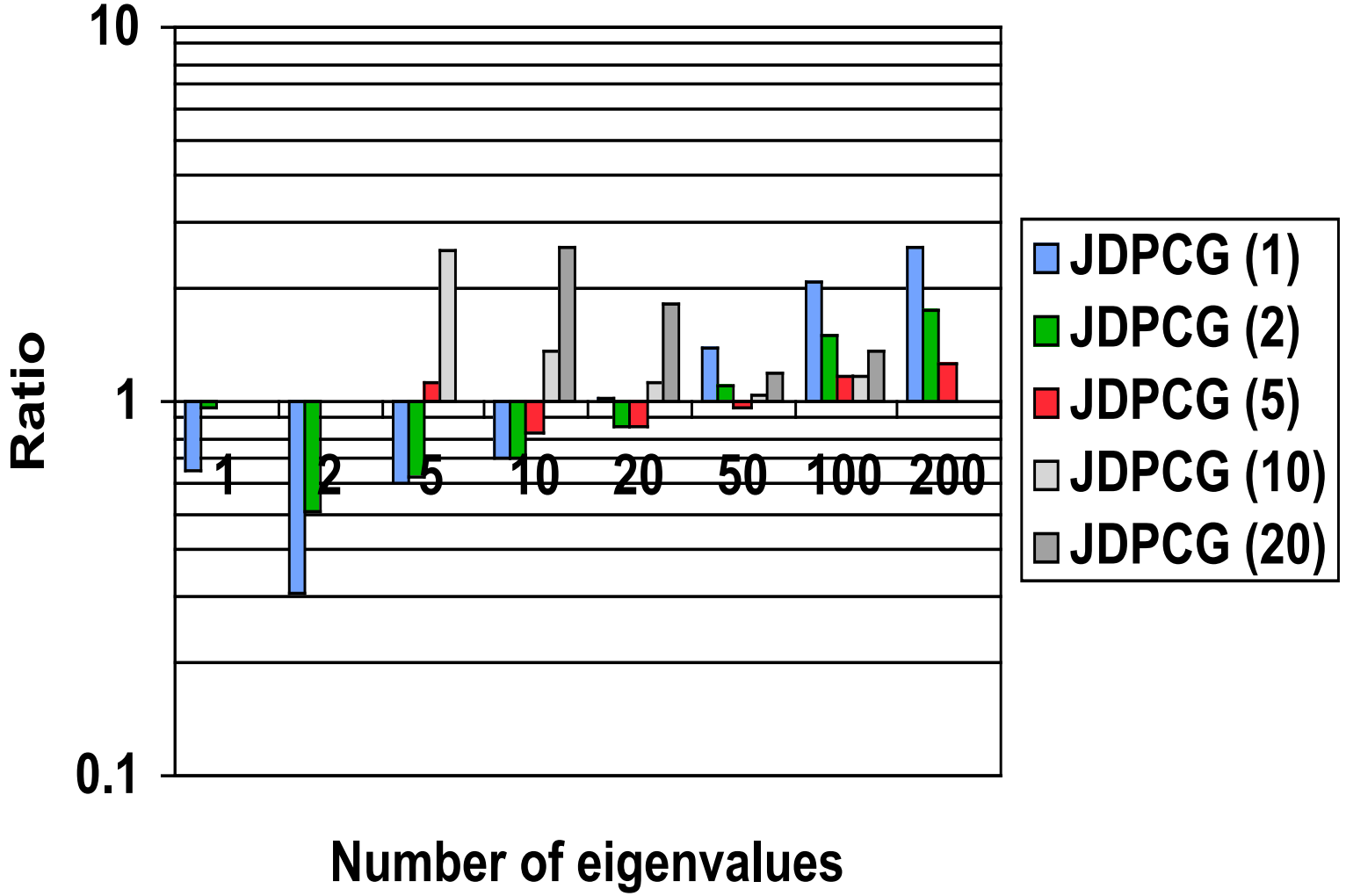
Relative Time vs ARPACK



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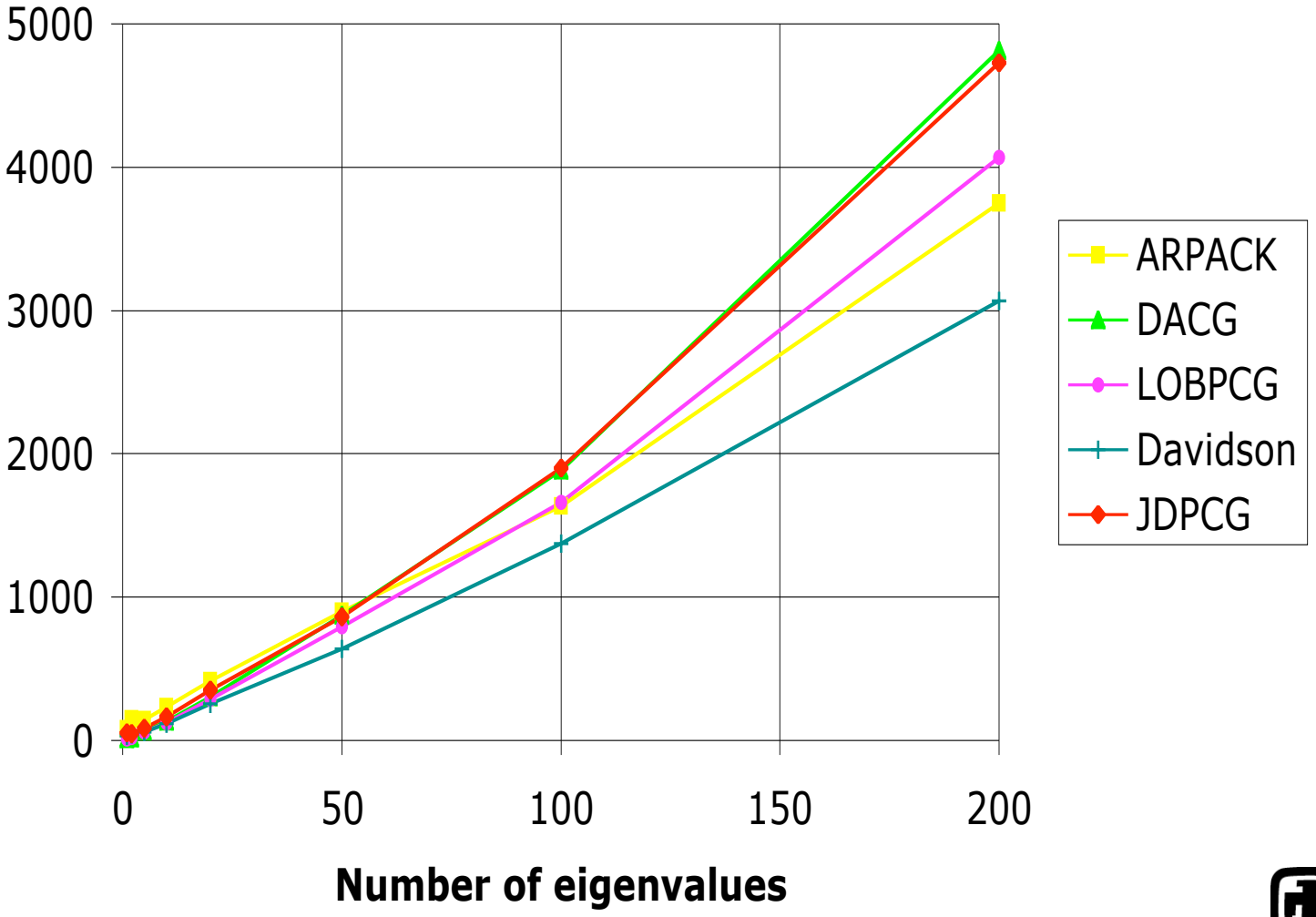
Time Summary

- **Preconditioner applications are not blocked.**



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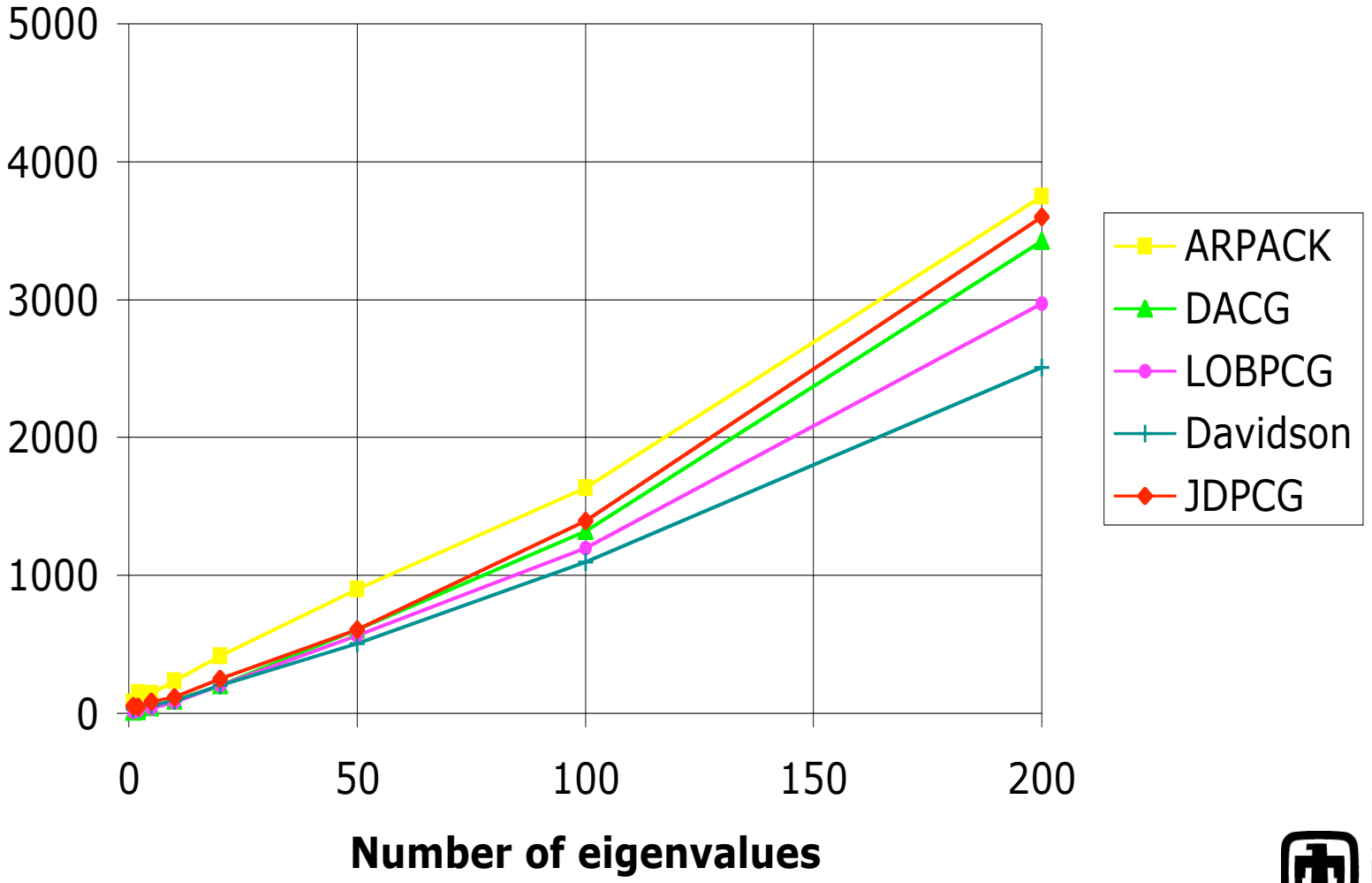
Time with Blocked Preconditioner

- **Speedup of 2 for preconditioner-vector applications**



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Memory Cost

Lanczos method:

- ncv (= 2*nev) vectors
- 3 vectors
- Arrays for $O(nev^2)$

Block DACG:

- nev vectors
- 8 blocks of vectors
- Arrays for $O(b^2)$

LOBPCG:

- nev vectors
- 10 blocks of vectors
- Arrays for $O(b^2)$

Davidson:

- ncv (= 2*nev) vectors
- 4 blocks of vectors
- Arrays for $O(nev^2)$

Jacobi-Davidson:

- ncv (= 2*nev) vectors
- 2*nev vectors
- 5 blocks of vectors
- Arrays for $O(nev^2)$

Size of block = b

Summary

Comments:

- Applications of preconditioner should be blocked.
- For this problem, Davidson is a good simple algorithm.
- For this problem, Jacobi-Davidson did not improve the performance.
- Ultimately, orthogonalization becomes the bottleneck.

Future work:

- Test the solvers on elasticity problems
- Evaluate the CMS method

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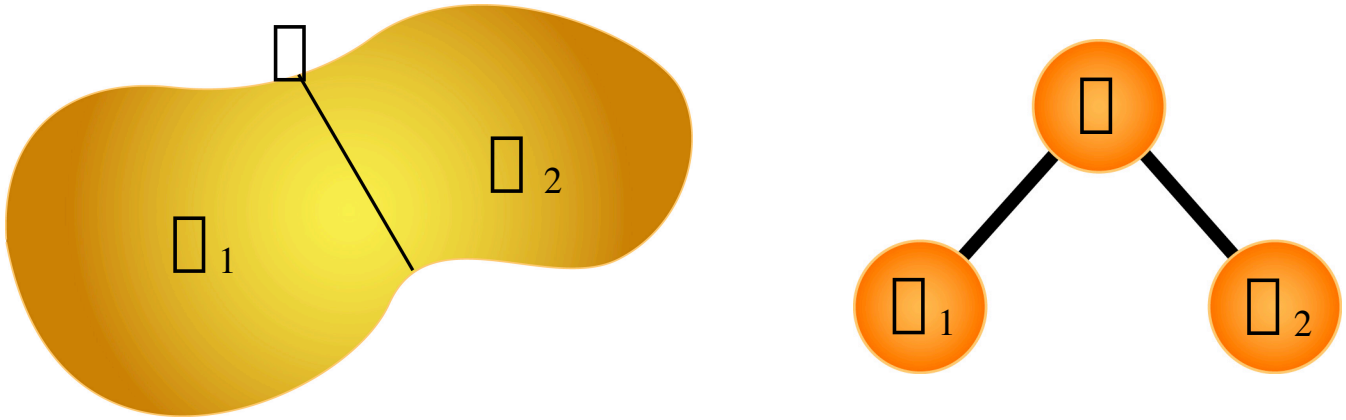
Component Mode Synthesis (CMS)

Idea: **Compute the first eigenmodes of a structure that can be subdivided into substructures on each of which the first eigenmodes are known.**



1. **Compute a few local eigenmodes in Ω_1**
2. **Compute a few local eigenmodes in Ω_2**
3. **Compute a few local eigenmodes on Γ**
4. **Approximate the global eigenmodes with the local modes**

Reference: W. Hurty (1965), R. Craig and M. Bampton (1968), F. Bourquin (1991)

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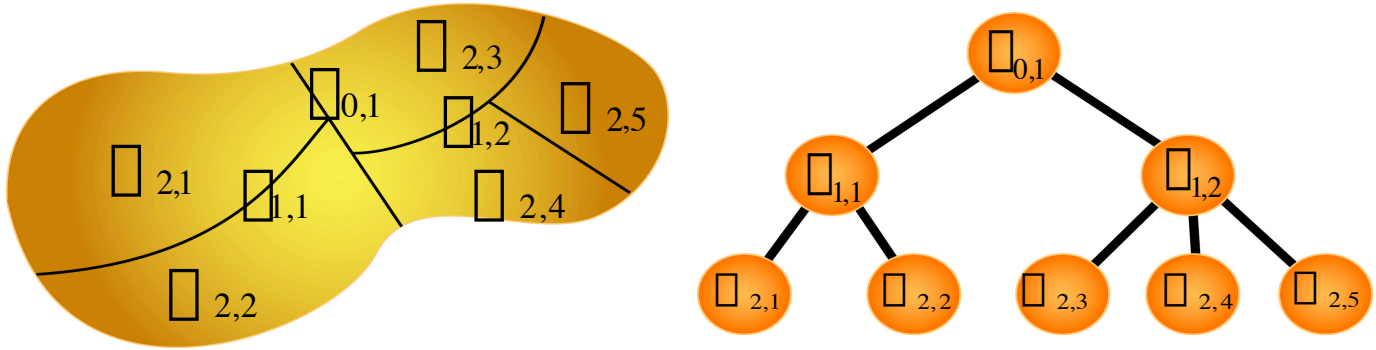
Component Mode Synthesis (CMS)

- **Automated MultiLevel Substructuring method (AMLS)**
  - **Apply the previous idea recursively**
  - **Use multilevel nested dissection to partition the domain**



Loop over the substructures

…

Solve a local generalized eigenproblem

…

…

Solve a coarse eigenproblem for synthesis

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Component Mode Synthesis (CMS)

- **Automated MultiLevel Substructuring method (AMLS)**

  - **For shells and plates (2D-like) problems, AMLS brings a major improvement in CPU time and memory costs over classical methods.**

    - ***Works of J. Bennighof and his group at UT Austin.***
    - ***Experiments of A. Kropp and D. Heiserer (BMW).***

  - **Very few 3D computations for real problems have been done !**

    - ***Work in progress (issues similar for a multifrontal solver)***