Solving Nonlinear Eigenproblems in Accelerator Cavity Design

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Overview

- Background
- Eigenvalue problem for RF cavity with external coupling
- Algorithms used
  - Second order Arnoldi (SOAR)
  - Nonlinear Arnoldi
  - Self consistent loop (SCL)
- Numerical examples
  - Linac Coherent Light Source RF-gun
  - Accelerating cavity for International Linear Collider
- Summary and Future work

DOE HEP SciDAC Project-
Electromagnetics System Simulations (ESS)

- *SLAC leads the* ***Electromagnetic Systems Simulation*** *(**ESS**) component in "Advanced Computing for 21st Century Accelerator Science and Technology" project*
  - Concentrates on developing **parallel tools** based on **unstructured grids** for the design, analysis, and optimization of complex electromagnetic components and systems in accelerators
  - Applies these tools to improve existing facilities, to design future accelerators, and to advance accelerator science
  - Collaborates with **SAPP/ISIC** collaborators to overcome **CS/AM Barriers** in solving challenging electromagnetic modeling problems that require **Large-scale simulations**

SciDAC
Scientific Discovery through Advanced Computing

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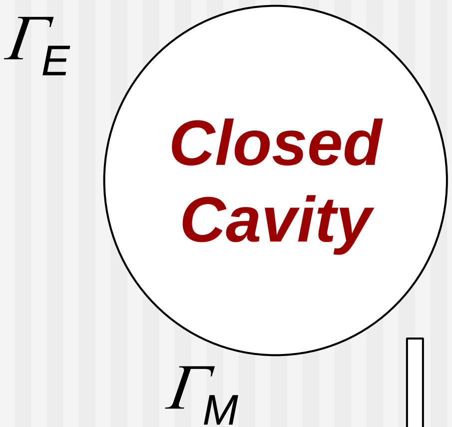
RF Cavity Eigenvalue Problem

Find frequency and field vector of normal modes:



"Maxwell's Eqns"

$$\nabla \times \nabla \times \mathbf{E} - k^2 \mathbf{E} = 0$$

$$n \times \mathbf{E} = 0 \quad \text{on } \Gamma_E$$

$$n \times \nabla \times \mathbf{E} = 0 \quad \text{on } \Gamma_M$$

Nedelec-type Element $\mathbf{E} = \sum_i x_i \mathbf{N}_i$

$$\mathbf{K}x = k^2 \mathbf{M}x$$

$$\mathbf{K}_{ij} = \int_\Omega (\nabla \times \mathbf{N}_i) \cdot (\nabla \times \mathbf{N}_j)\, d\Omega$$

$$\mathbf{M}_{ij} = \int_\Omega \mathbf{N}_i \cdot \mathbf{N}_j \, d\Omega$$

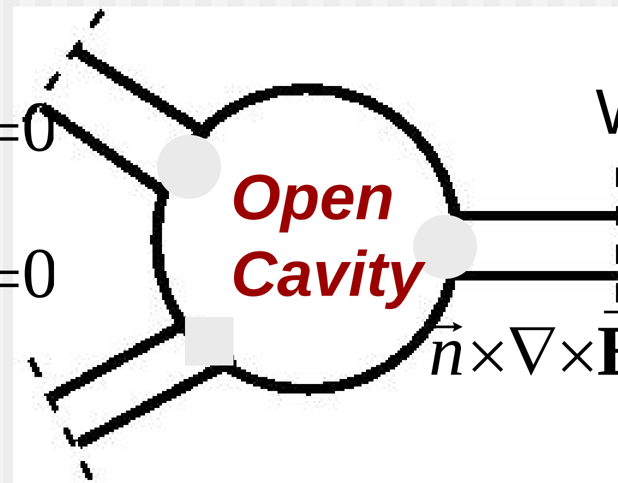
Cavity with External Coupling

Waveguide BC

$$\vec{n}\times\nabla\times\vec{\mathbf{E}}+i\sqrt{k^2-k_{c3}^2}\,\vec{n}\times\vec{n}\times\vec{\mathbf{E}}=0$$

$$\vec{n}\times\nabla\times\vec{\mathbf{E}}+i\sqrt{k^2-k_{c2}^2}\,\vec{n}\times\vec{n}\times\vec{\mathbf{E}}=0$$

Waveguide BC



Waveguide BC

$$\vec{n}\times\nabla\times\vec{\mathbf{E}}+i\sqrt{k^2-k_{c1}^2}\,\vec{n}\times\vec{n}\times\vec{\mathbf{E}}=0$$

- Vector wave equation with waveguide boundary conditions can be modeled by a **non-linear eigenvalue problem**

$$\mathbf{K}x + i\sum_j \sqrt{k^2 - k_{cj}^2}\,\mathbf{W}_j x = k^2\mathbf{M}x$$

With $(\mathbf{W}_j)_{ik} = \int_\Gamma (n \times \mathbf{N}_i)\cdot(n \times \mathbf{N}_k)\,d\Gamma$

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Quadratric Eigenvalue Problem

- Consider only one mode propagating in the waveguides
- Nonlinear eq. reduces to quadratic form:

$$\mathbf{K}x + i\sqrt{k^2 - k_c^2}\mathbf{W}x = k^2\mathbf{M}x$$

$$\lambda = \sqrt{k^2 - k_c^2}$$

$$\lambda^2\mathbf{M}x - i\lambda\mathbf{W}x + (k_c^2\mathbf{M} - \mathbf{K})x = 0$$

Second-Order Krylov Space
(Bai et al, 05)

Krylov subspace:

$$\mathcal{K}_n(\mathbf{A}, u) = span\{u, \mathbf{A}u, ..., \mathbf{A}^{n-1}u\}$$

Given matrix $\mathbf{A}$ and $\mathbf{B}$, vector u,

$$\begin{aligned} r_0 &= u \\ r_1 &= \mathbf{A}r_0 \\ r_j &= \mathbf{A}r_{j-1} + \mathbf{B}r_{j-2} \end{aligned}$$

the sequence r_0, r_1, ..., r_{n-1} is called a second-order *Krylov* sequence.

$$\mathcal{G}_n(\mathbf{A}, \mathbf{B}, u) = span\{r_0, r_1, ..., r_{n-1}\}$$

Applying Second Order Arnoldi

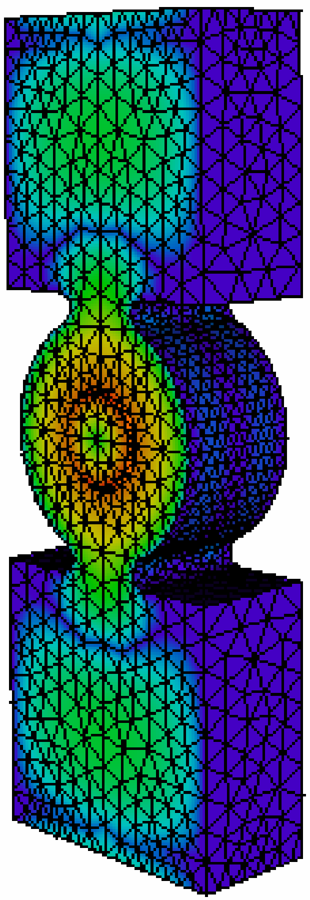
Given $(\lambda^2 \mathbf{M} + \lambda \mathbf{D} + \mathbf{K})x = 0,\ \begin{matrix} \mathbf{A} = -\mathbf{M}^{-1}\mathbf{D} \\ \mathbf{B} = -\mathbf{M}^{-1}\mathbf{K} \end{matrix}$

- Generate orthonormal basis $\mathbf{Q}_n$ of second-order Krylov subspace $\mathcal{G}_n(\mathbf{A}, \mathbf{B}, u)$
- Compute projection matrices $\mathbf{M}_n = \mathbf{Q}_n^T \mathbf{M} \mathbf{Q}_n,\ \mathbf{D}_n = \mathbf{Q}_n^T \mathbf{D} \mathbf{Q}_n,\ \mathbf{K}_n = \mathbf{Q}_n^T \mathbf{K} \mathbf{Q}_n$
- Solve the QEP: $(\theta^2 \mathbf{M}_n + \theta \mathbf{D}_n + \mathbf{K}_n)g = 0$
- Compute Ritz pairs $(\theta, z) = \left(\theta, \frac{\mathbf{Q}_n g}{||\mathbf{Q}_n g||_2}\right)$
- Test for convergence

SOAR directly applies to QEP, converges faster

Single Cavity coupled to External Waveguides

Test Case

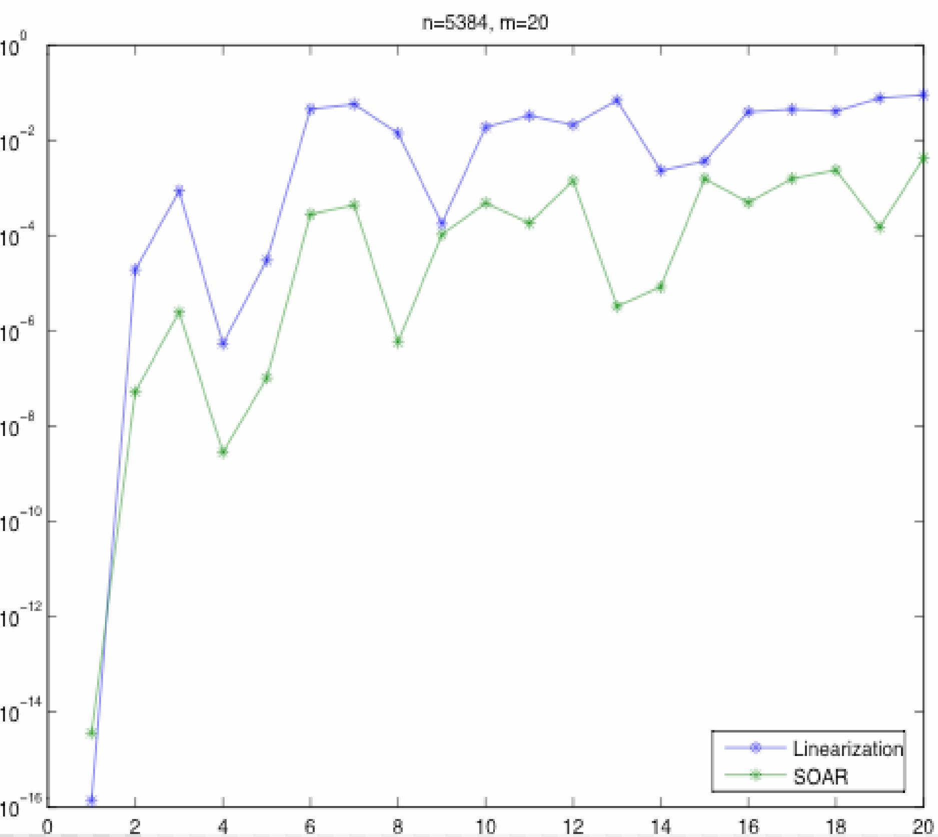


Parallel SOAR implemented into SLAC's parallel 3D finite element eigensolver Omega3P

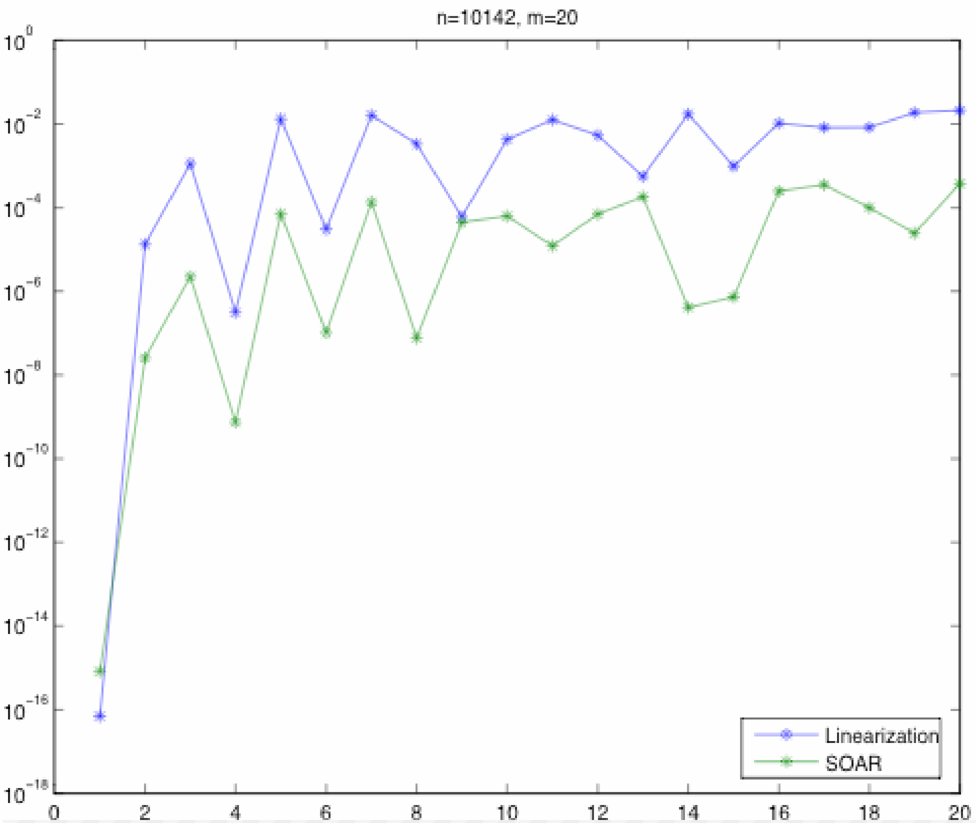
- External waveguides terminated with waveguide BC (only 1 propagating mode)
- Results agree remarkably with experiments
  - Frequency=9.396GHz
  - External Q=178 $Q_{ext} = \frac{Re(f)}{2 \times Im(f)}$

Linearization versus SOAR

N=5384



N=10142



Nonlinear Arnoldi Method
(Voss et al. '02,'03)

$$\mathbf{T}(\lambda)x = 0,\ \lambda = k^2 \text{ and}$$

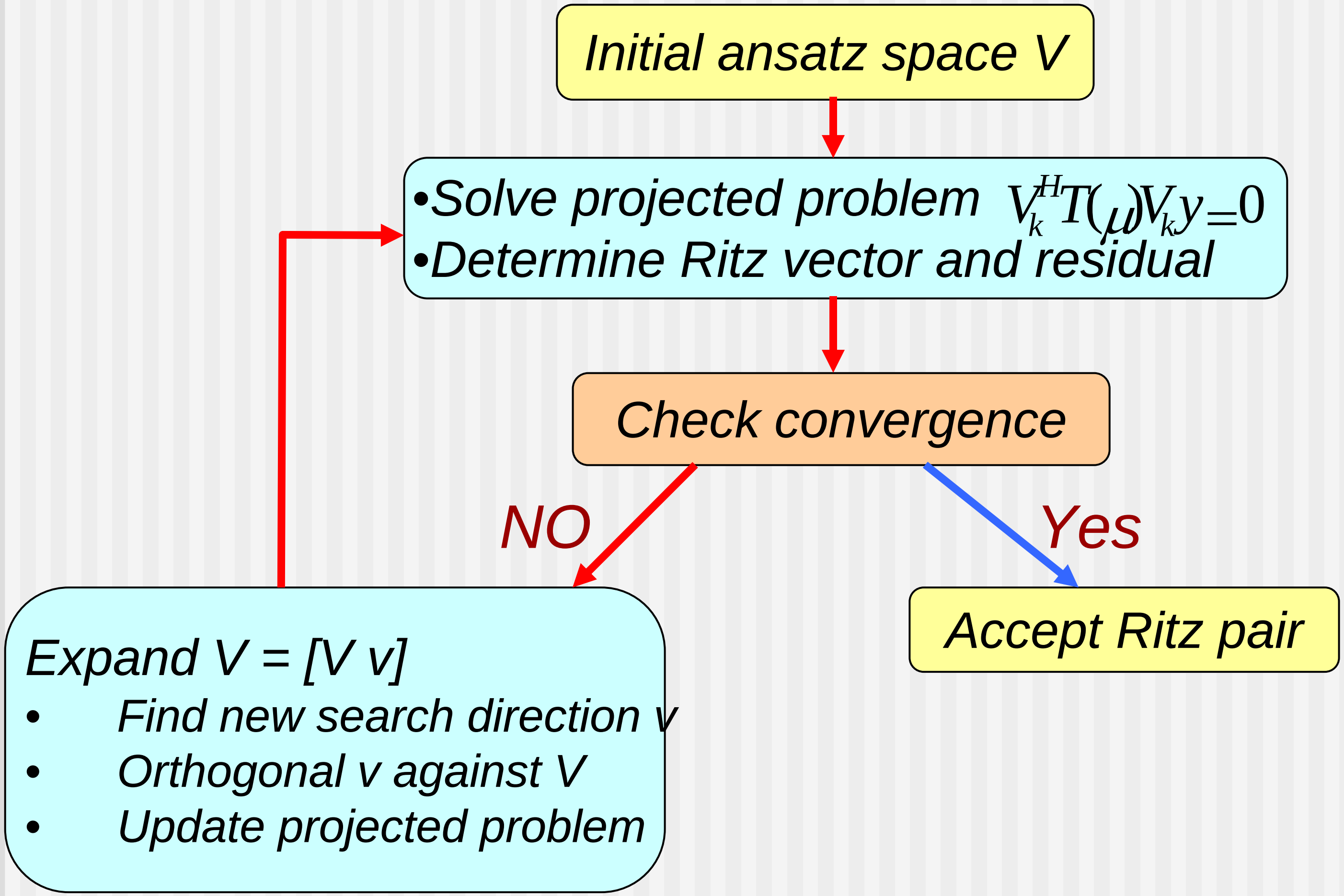
$$\mathbf{T}(\lambda) = \mathbf{K} + i\sum_j \sqrt{\lambda - k_{cj}^2}\,\mathbf{W}_j - \lambda\mathbf{M}$$

- An iterative projection method
- Eigenvalues are determined one after another
- New search direction is formed via the residual inverse iteration (Neumaier '85)

$$v = \mathbf{T}(\sigma)^{-1}\mathbf{T}'(\hat{\lambda})\hat{x}$$

  - σ is the shift
  - $T(\sigma)^{-1}$ can be treated as preconditioner
  - The projected nonlinear problem is formed through Arnoldi-type procedure

Basic Algorithm of Nonlinear Arnoldi



Solve & Update projected problems

- Projected problems are small and dense
- Methods (nonlinear eigensolvers)
  - Method of successive linear problem (Ruhe '73)
  - (Residual) inverse iteration method
- Update of projected problem:

$$\mathbf{T}(\lambda) = \mathbf{K} + i\sum_j \sqrt{\lambda - k_{cj}^2}\mathbf{W}_j - \lambda\mathbf{M} = \sum_j f_j(\lambda)\mathbf{C}_j$$

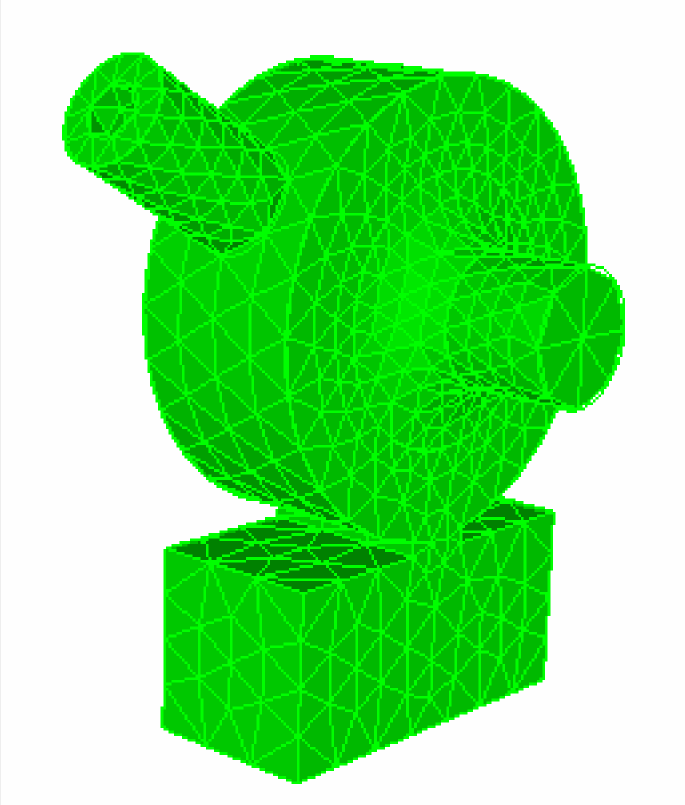
Then

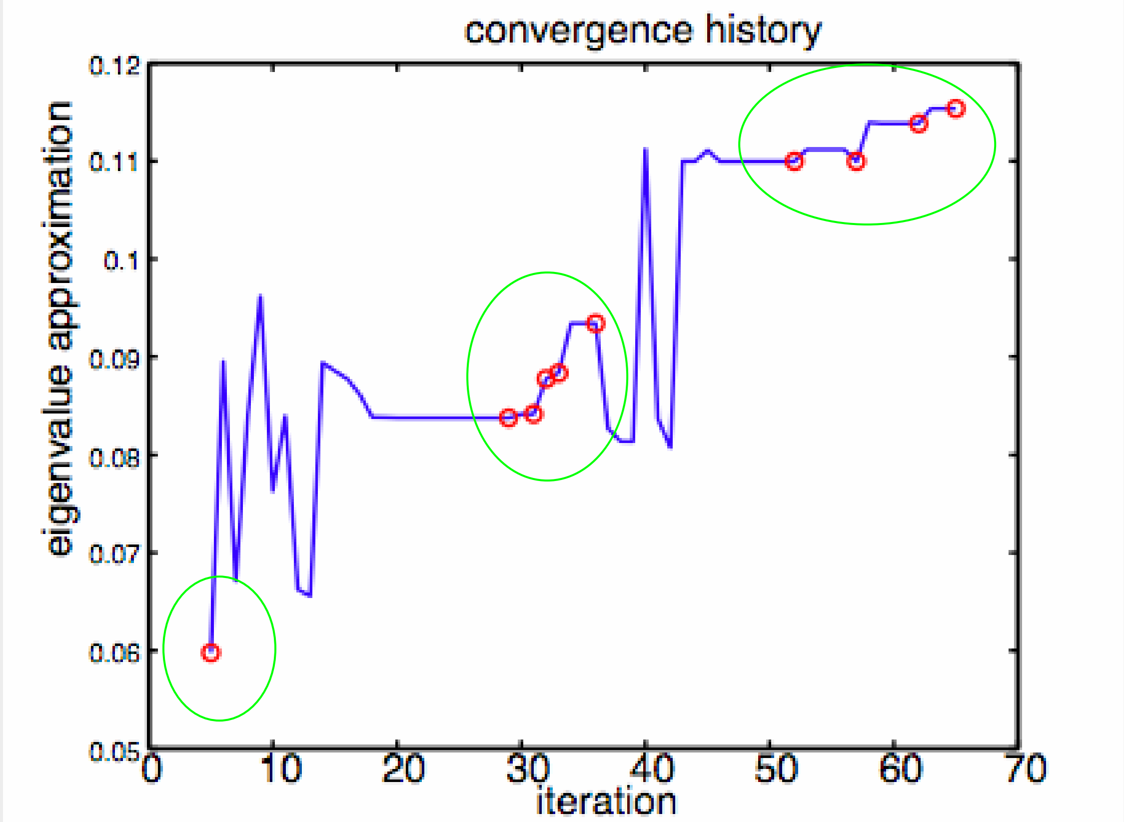
$$\mathbf{T}_{V_k}(\lambda) = \sum_j f_j(\lambda) V_k^H \mathbf{C}_j V_k = \sum_j f_j(\lambda)\mathbf{C}_{j,k}$$

and matrices C_j can be updated according to

$$\mathbf{C}_{j,k} = \begin{pmatrix} \mathbf{C}_{j,k-1} & V_{k-1}^H C_j v \\ v^H \mathbf{C}_j V_{k-1} & v_H C_j v \end{pmatrix}$$

Testing Example - RF-gun Cavity with Two Ports





- *Eigenvalues are typically clustered in our problems.*
- *To find an eigenvalue in the next cluster requires more efforts.*
- *May miss eigenvalues in the calculatioon!*

Self Consistent Loop (SCL)

$$\mathbf{K}x + i\sum_j \sqrt{k^2 - k_{cj}^2}\mathbf{W}_j x = k^2\mathbf{M}x$$

- Ignore the waveguide terms first and solve

$$\mathbf{K}x = k^2\mathbf{M}x$$

- Loop until converge (often in 3 iterations)
  - Use the ***k*** computed in the previous step and evaluate $\hat{\mathrm{K}} = \mathrm{K} + i\sum_j \sqrt{k^2 - k_{cj}^2}\mathbf{W}_j$
  - Then solve $\hat{\mathbf{K}}x = k^2\mathbf{M}x$
- No convergence proof but often converges

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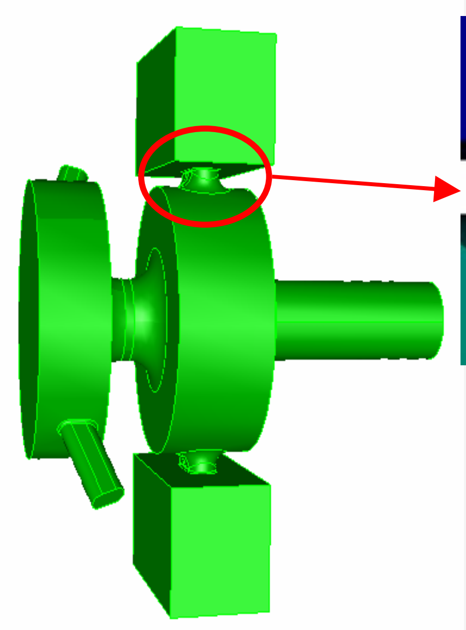
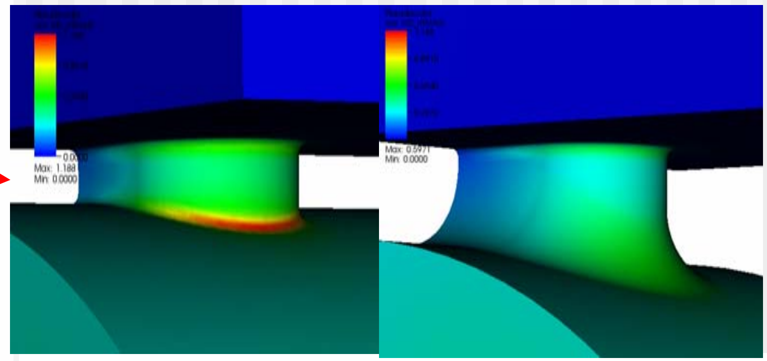
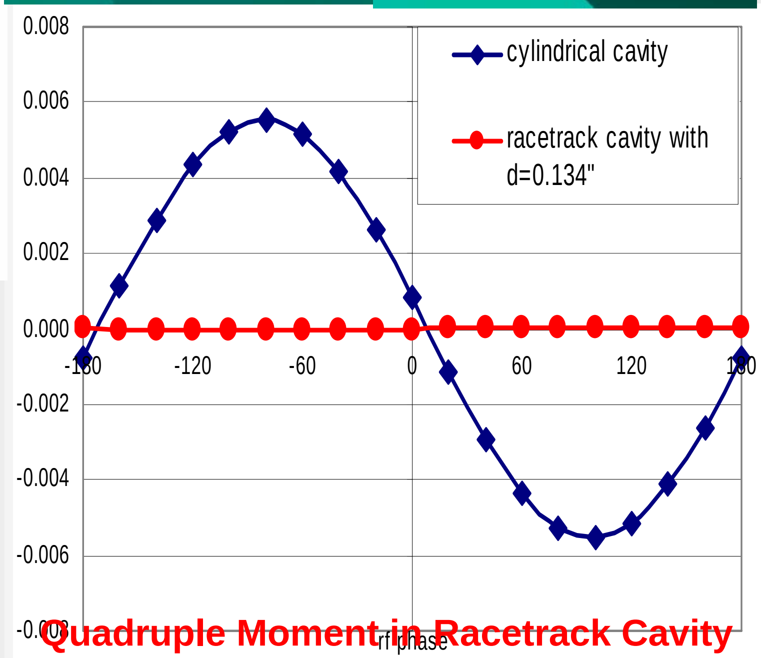
Linac Coherent Light Source (LCLS) RF-Gun Design







Omega3P with SOAR/SCL is used for computing frequency, Q_0, and $Q_{external}$

New Design

- Dual RF feeds: Eliminate dipole modes
- Larger rounding of Iris: Reduce pulsed heating
- Racetrack cell shape: Minimize quadruple mode

Typical run:

NDOFs: 3.2 million

NNZ: 440 million

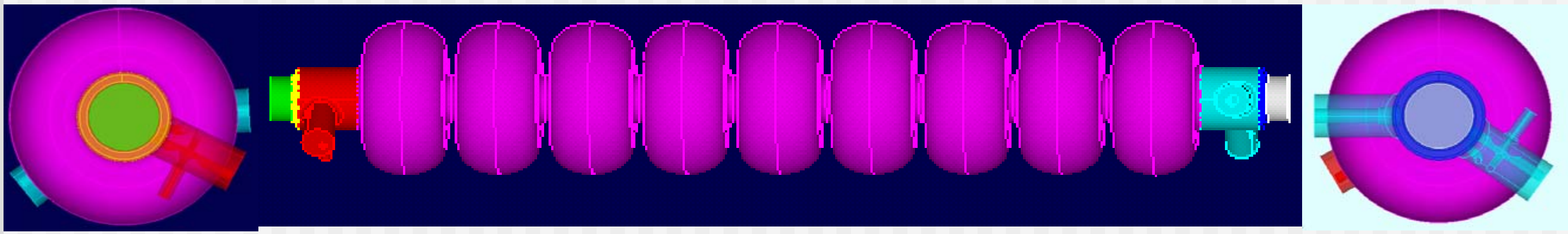
NCPUs: 256/32

Memory: 400GB

Time: 2 hours

for 2 eigen-modes

Accelerating Cavity for International Linear Collider (ILC)



- ❑ 9-cell superconducting cavity coupled to one input coupler and two Higher-Order-Mode couplers.
- ❑ All couplers terminate in coax TEM mode with the same k_c

$$\mathbf{K}x + i\sum_j \sqrt{k^2 - k_{cj}^2}\,\mathbf{W}_j x = k^2\mathbf{M}x \Longrightarrow \mathbf{K}x + i\sqrt{k^2 - k_c^2}\sum_j \mathbf{W}_j x = k^2\mathbf{M}x$$

$$\Downarrow$$

$$\lambda^2\mathbf{M}x - i\lambda\sum_j \mathbf{W}_j x + (k_c^2\mathbf{M} - \mathbf{K})x = 0$$

- ❑ SOAR is used mainly
- ❑SCL is used when beampipes are open

<u>Computational Challenges</u>

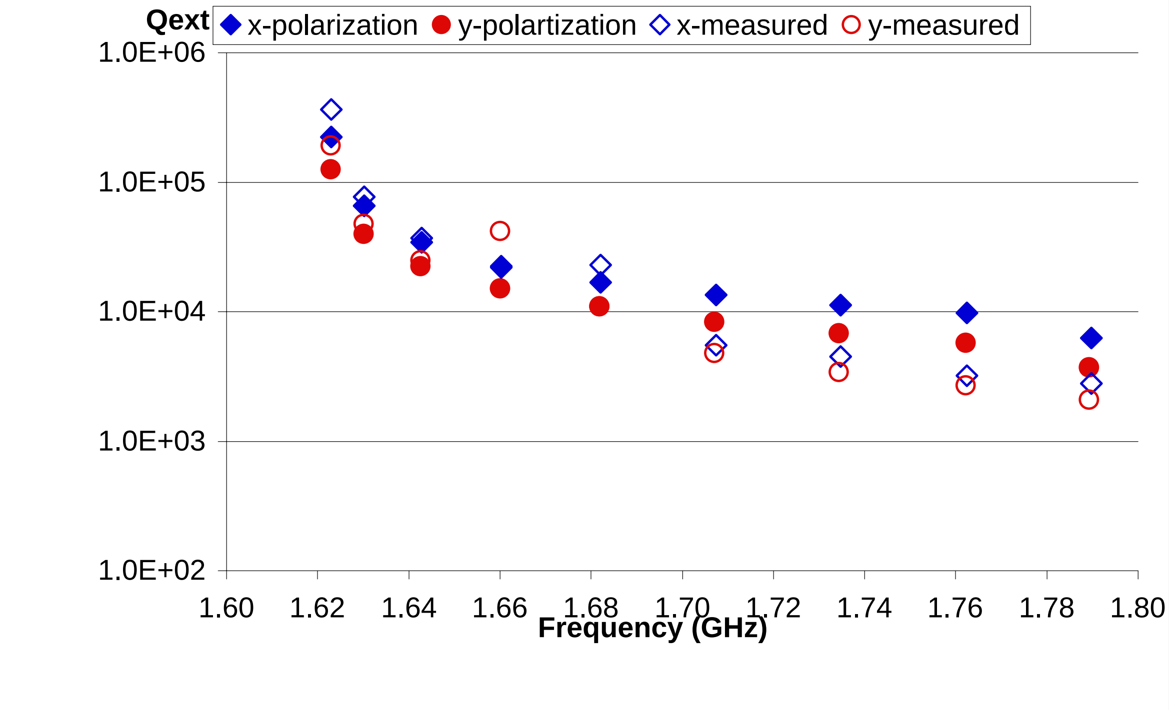
- *Large mesh to resolve fine features accurately*
- *Many tightly clustered interior complex eigenvalues*

ILC Cavity Simulation

Numerical results show good agreement with measured data on frequency f and Q_{ext} of 1^{st} band dipole modes

$$Q_{ext} = \frac{Re(f)}{2 \times Im(f)} \text{ where } f = \frac{c}{2\pi}k$$

Typical run:
NDOFs: 3.2 million
NNZ: 132 million
NCPUs: 768/96
Memory: 300GB
Time: 150s per eigen-modes



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Summary

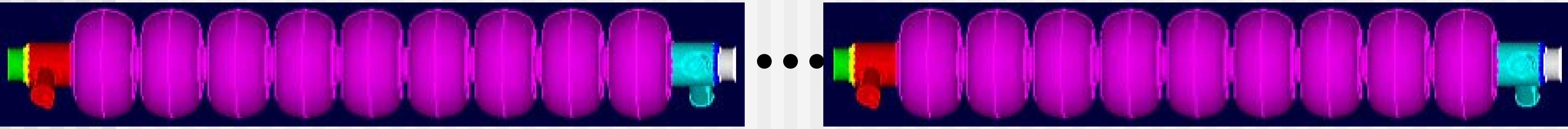
- SOAR and SCL
  - Successfully applied in accelerator cavity design for simulating open cavities
- Nonlinear Arnoldi
  - Initial results are promising
  - Need further study in finding multiple eigenvalues
  - To be implemented in Omega3P in parallel

Future Work

- Faster and robust methods for solving multiple waveguide modes:

$$\mathbf{K}x + i\sqrt{k^2 - k_{c1}^2}\mathbf{W}_1 x + i\sqrt{k^2 - k_{c2}^2}\mathbf{W}_2 x = k^2\mathbf{M}x$$

- Model chain of ILC cavities
  - More nonlinear terms
  - Much bigger systems



Up to 12 cavities connected together

Thanks!

Residual Inverse Iteration

Start from approximate eigenvalue σ, x_1, e with $e^H x_1 = 1$

for $\ell = 1, 2, \ldots$ until convergence **do**

solve $e^H T(\sigma)^{-1} T(\lambda_{\ell+1}) x_\ell = 0$ for $\lambda_{\ell+1}$

compute the residual $r_\ell = T(\lambda_{\ell+1}) x_\ell$

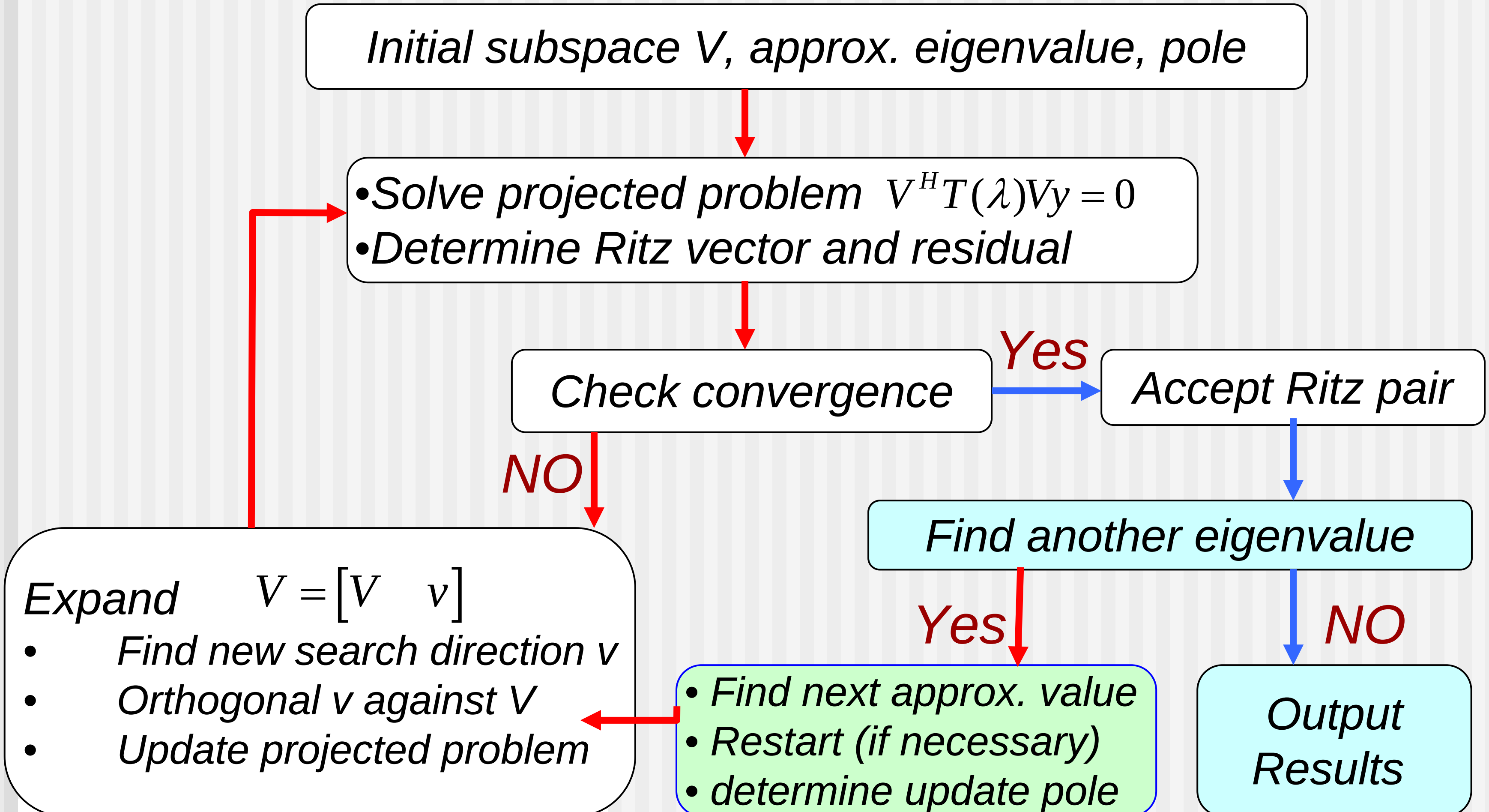
solve $T(\sigma) d_\ell = r_\ell$ for d_ℓ

set $y_{\ell+1} = x_\ell - d_\ell$

normalize $x_{\ell+1} = y_{\ell+1} / e^H y_{\ell+1}$

end for

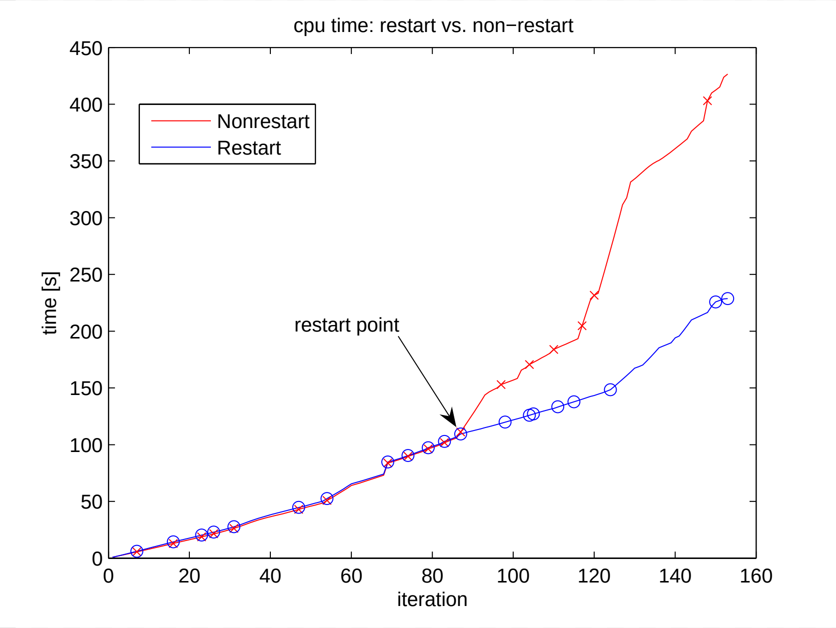
Algorithm with additional features

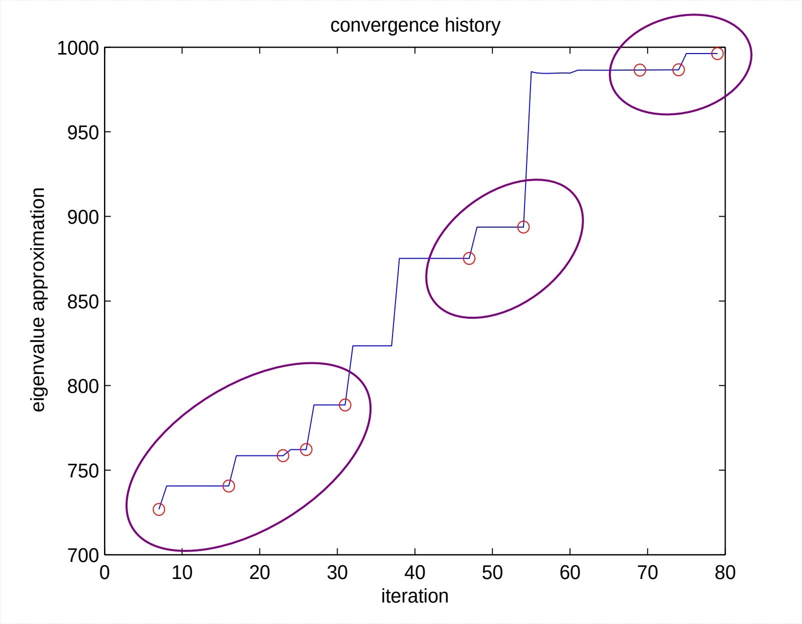


Example I - TwoTerms

$$T(\lambda)x = \left(K + i\sqrt{\lambda^2 - \lambda_0^2}W_0 + i\sqrt{\lambda^2 - \lambda_1^2}W_1 - \lambda^2 M\right)x = 0$$

N = 7791





Second Order Arnoldi (SOAR)

Inputs: $\mathbf{A}, \mathbf{B}, \mathbf{u} \neq \mathbf{0}, n \geq 1$

Output: an orthonormal basis of $\mathcal{G}_n(\mathbf{A}, \mathbf{B}; \mathbf{u})$: $\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_n$

$\mathbf{q}_1 = \mathbf{u}/\|u\|$ — basis vector

$\mathbf{p}_1 = \mathbf{0}$ — auxiliary vector

for $j = 1, 2, \ldots, n$ do

  $\mathbf{r} = \mathbf{A}\mathbf{q}_j + \mathbf{B}\mathbf{p}_j$

  $\mathbf{s} = \mathbf{q}_j$

  for $i = 1, 2, \ldots, j$ do — *orthogonal wrt q-vectors*

    $t_{ij} = \mathbf{q}_i^T \mathbf{r}$

    $\mathbf{r} := \mathbf{r} - \mathbf{q}_i t_{ij}$

    $\mathbf{s} := \mathbf{s} - \mathbf{p}_i t_{ij}$

  $t_{j+1,j} = \|\mathbf{r}\|_2$

  if $t_{j+1,j} = 0$, stop — deflation or breakdown

  $\mathbf{q}_{j+1} = \mathbf{r}/t_{j+1,j}$ — basis vector

  $\mathbf{p}_{j+1} = \mathbf{s}/t_{j+1,j}$ — auxiliary vector

Comparison of Methods

- *On NERSC's IBM SP, ILC cavity model requires:*
- *NDOFs=3.2million, NCPUs=768, Memory=300GB*
- *WSMP for solving sparse linear systems*

Method	# of Modes	Wall clock
SOAR	18	2634s
SCL	1	4800s

- SOAR is able to solve multiple eigen-pairs with one sparse direct factorization
- Using SCL we have to solve modes one-by-one

SOAR Implementation using ITL

- Iterative Template Library designed for maximal reuse
  - *Linear algebra operations interface to different software packages(BLAS, μBLAS, MTL, A++/P++)*
  - *Krylov subspace iterative methods for linear systems*
  - *Interface to sparse direct solvers (WSMP, SuperLU, MUMPS)*
  - *Serial and parallel algorithms share the same code with different interfaces*
- SOAR implementation using ITL has almost one-to-one correspondence between algorithm description and C++ code
- Shift-and-Invert spectral transformation included

SOAR versus Arnodi (Linearization)

SOAR in matrix notation:

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{I} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{Q}_n \\ \mathbf{P}_n \end{pmatrix} = \begin{pmatrix} \mathbf{Q}_{n+1} \\ \mathbf{P}_{n+1} \end{pmatrix} \hat{\mathbf{T}}_n$$

Arnodi in matrix notation:

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{I} & \mathbf{0} \end{pmatrix} \mathbf{V}_n = \mathbf{V}_{n+1} \hat{\mathbf{H}}_n$$

Difference: Orthonormality