Solving Large Scale Nonlinear Eigenvalue Problems in Next-Generation Accelerator Design

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International Linear Collider (ILC)

*http://www.linearcollider.org/*

The ILC is a proposed new electron-positron collider that would allow physicists to answer compelling questions on identity of dark matter to the existence of extra dimensions. In the ILC's design, two facing linear accelerators, each 20 kilometers long, accelerate electrons and positrons to TeV energy using superconducting accelerating cavities.
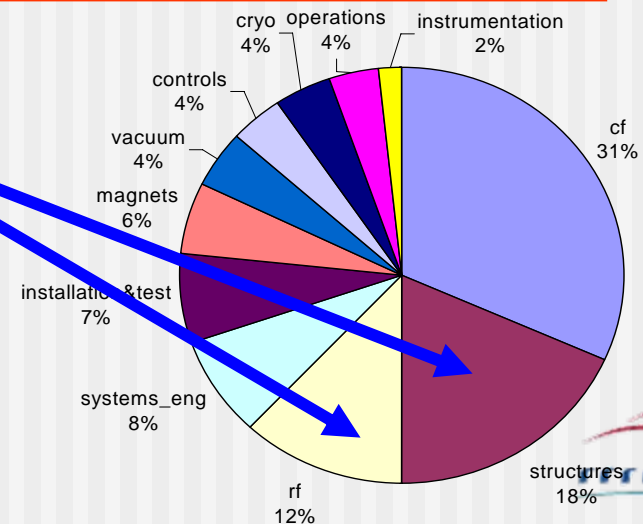
The Global Design Effort will establish the design of the ILC, focusing the efforts of hundreds of accelerator scientists and particle physicists in North America, Europe and Asia.
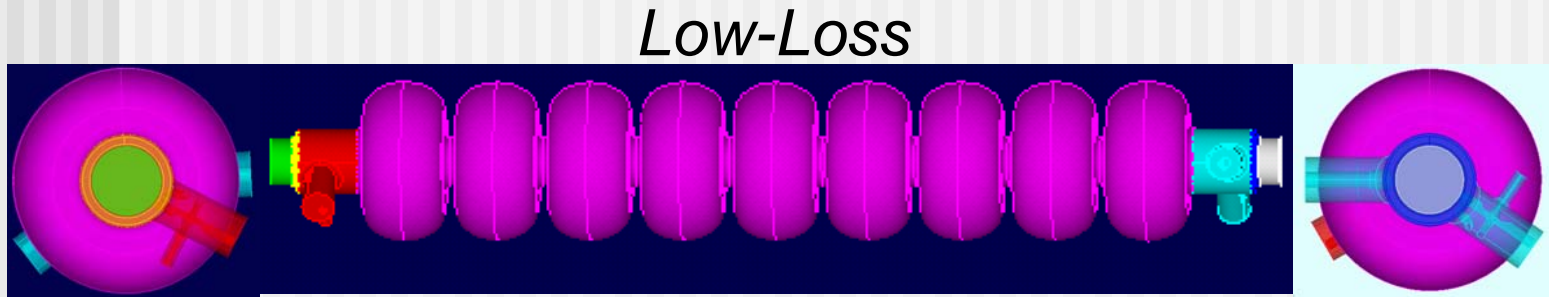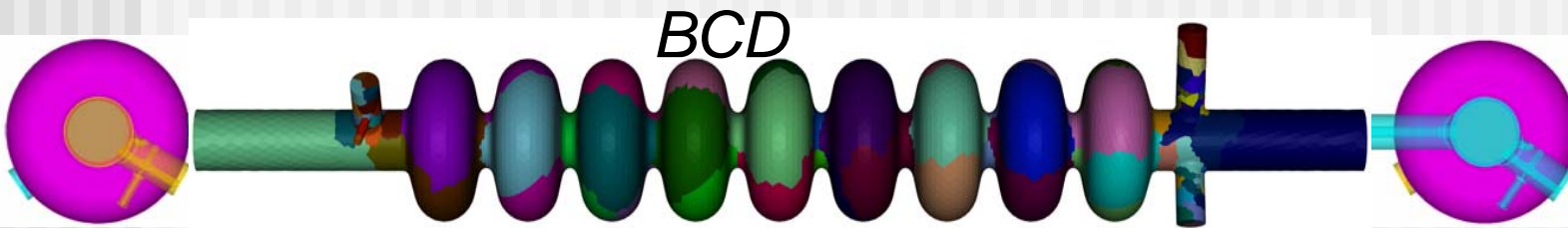
International Linear Collider
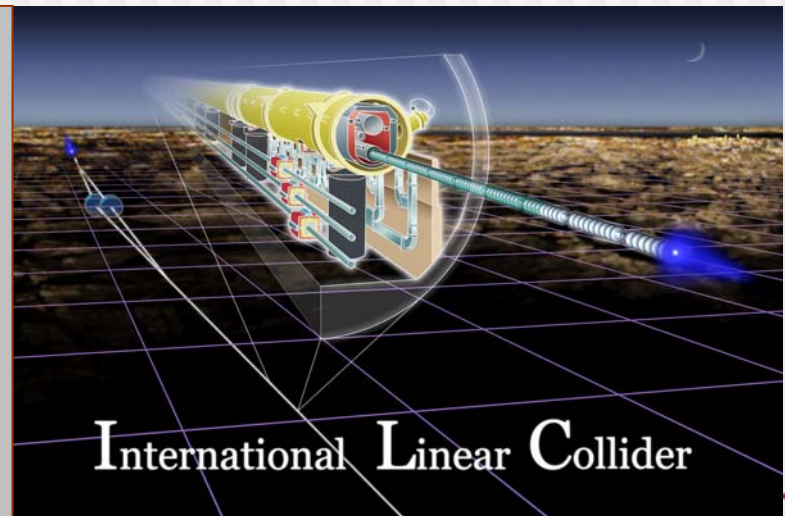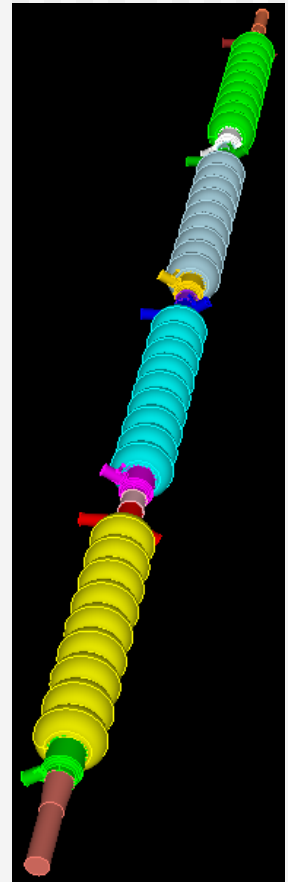
ILC Superconducting Main Linac
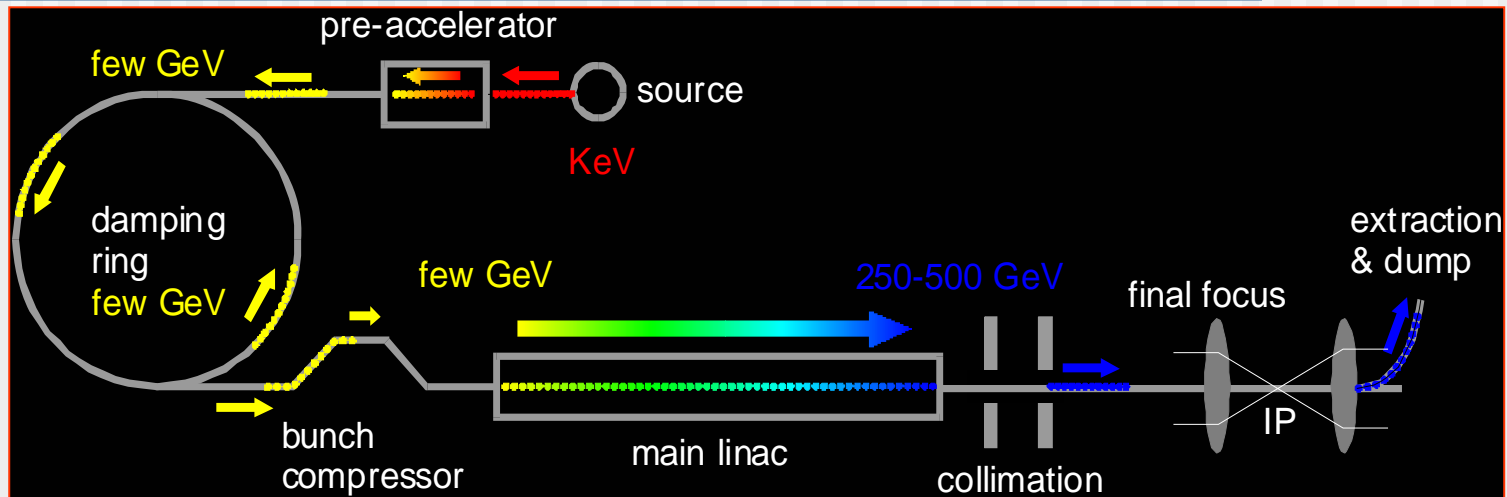
SRF Main Linac constitutes the heart of the accelerator at 30% of its total cost & consists of 20,000 SRF cavities to accelerate the beams to 0.5 TeV energy

Various ILC Cavities

BCD

STF1

Low-Loss

ICHIRO

SST

ILC Cyromodule and RF Unit

8-cavity Cyromodule

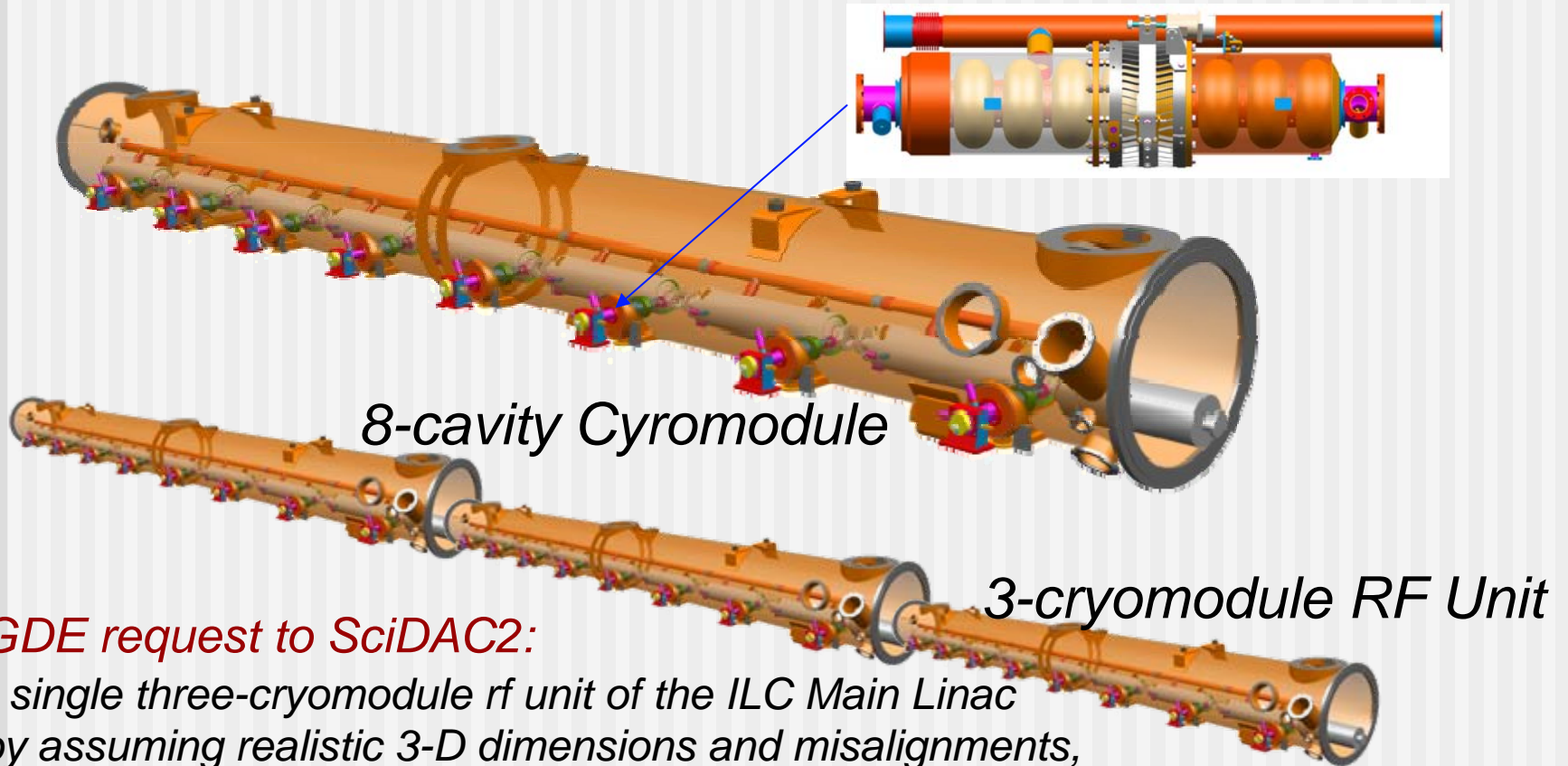*3-cryomodule RF Unit*

ILC GDE request to SciDAC2:

*For a single three-cryomodule rf unit of the ILC Main Linac
and by assuming realistic 3-D dimensions and misalignments,
calculate multi-bunch beam dynamics effects, including wakefields and HOM excitations.*

Outline of this talk

1. THE NEP

2. Initial approximations and ordering

3. NRRIT (Nonlinear Arnoldi Method)

4. Numerical experiments

THE NEP

- $T(\lambda)x = 0$, where

$$T(\lambda) = K - \lambda M + \mathbf{i} \sum_{j=1}^{p} \sqrt{(\lambda - \sigma_j^2)}\, W_j,$$

and K, M and W_j are $N \times N$ real symmetric,
$\quad K \geq 0$ and $M > 0$.
$\quad \sigma_j$ are given nonnegative scalars – cutoff values, $\mathbf{i} = \sqrt{-1}$.

- derived from a Nedelec-type FE discretization of the frequency domain Maxwell's equation with waveguide BCs [ISH95, KFG+06, Lee05a, Lee05b]

- Future: cavitiy with waveguide coupling for multiple waveguide modes

$$T(\lambda) = K - \lambda M + \mathbf{i} \sum_{j=1}^{p} \sqrt{(\lambda - \sigma_j^2)}\, W_j^{\text{TE}} + \mathbf{i} \sum_{j=1}^{p} \frac{\lambda}{\sqrt{(\lambda - \sigma_j^2)}}\, W_j^{\text{TM}}$$

Desired eigenvalues

- Let $\kappa = \sqrt{\lambda}$,

$$\text{resonant frequency} = f(\kappa) = \frac{c}{2\pi} \cdot \text{Re}(\kappa)$$

and

$$\text{external } Q_e\text{-value} = Q_e(\kappa) = \frac{1}{2} \cdot \frac{\text{Re}(\kappa)}{\text{Im}(\kappa)},$$
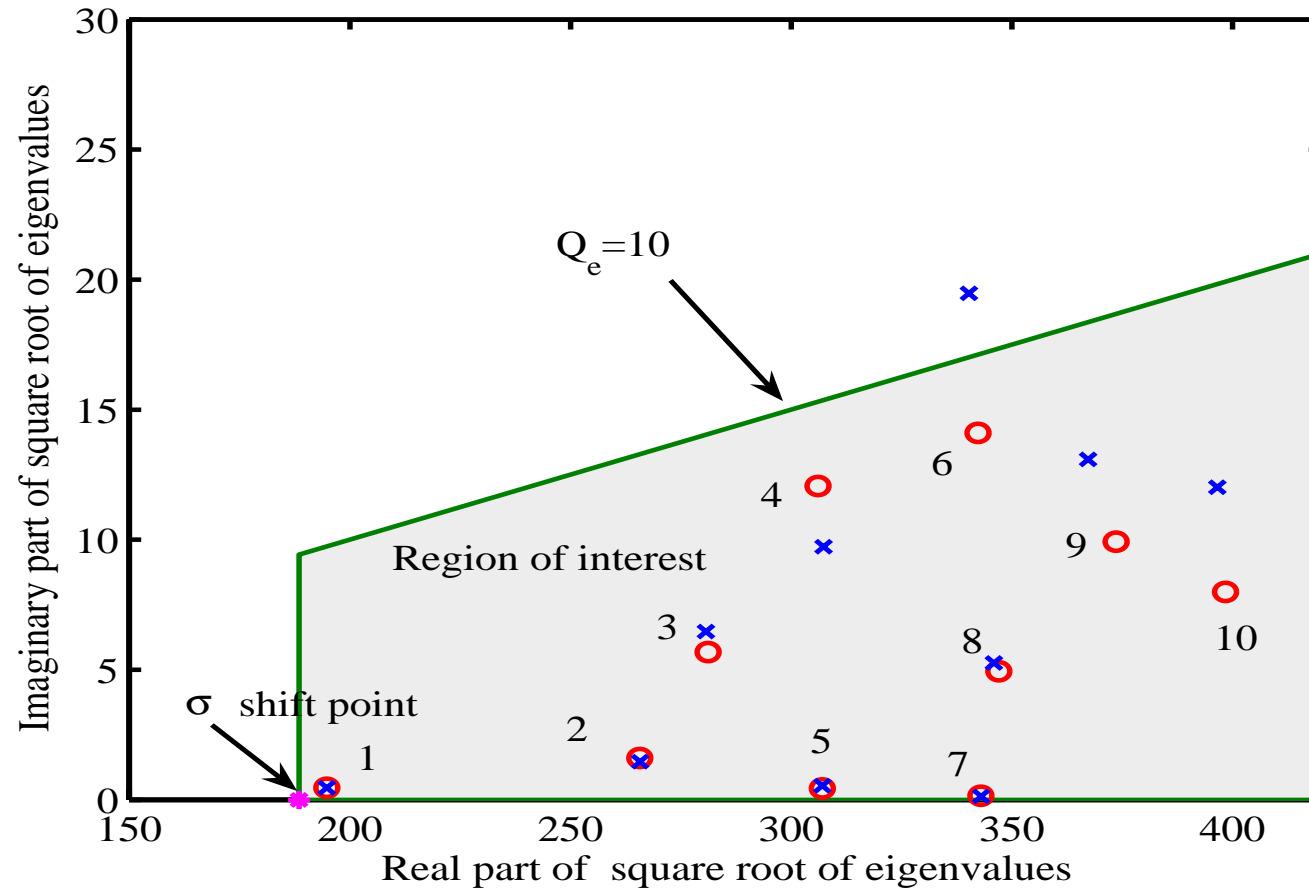
$c = 3 \times 10^8 m/s$, the speed of light in vacuum

- The external Q_e-values measure the electromagnetic coupling between the cavity and waveguide, characterize the energy loss.

- Seek eigenvalues λ satisfying

$$\begin{cases} \kappa = \sqrt{\lambda} \text{ is close to the shift value } \sigma_0 = \frac{2\pi}{c} f_0 \text{ and} \\ \lambda \in \mathcal{D} = \{\lambda \mid \lambda = \kappa^2, \ \text{Re}(\kappa) > \sigma_0, \ \text{Im}(\kappa) > 0 \text{ and } Q_e(\kappa) > \widehat{Q_e}\}, \end{cases}$$

where f_0 and $\widehat{Q_e} > 1$ are prescribed.

Desired eigenvalues

○: "exact" eigenvalues;   ×: initial approximations

Initial approximation/ordering

- The first order truncation:

$$T(\lambda) \approx T(\lambda_0) + (\lambda - \lambda_0)T'(\lambda_0)$$
$$\equiv \widehat{K}(\lambda_0) - \lambda\widehat{M}(\lambda_0),$$
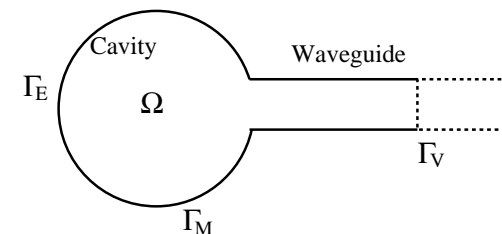
- Initial approximations:

$$\text{selected eigenpairs } (\theta_\ell, v_\ell) \text{ of } (\widehat{K}(\sigma_0^2), \widehat{M}(\sigma_0^2))$$

- Ordering:

$$|\theta_1^{1/2} - \sigma_0| \leq |\theta_2^{1/2} - \sigma_0| \leq \cdots \leq |\theta_n^{1/2} - \sigma_0|.$$

- Example:

$$\left[K - \lambda M + \mathbf{i}\sqrt{(\lambda - \sigma_1^2)}\, W_1\right] x = 0.$$

NRRIT

Nonlinear Rayleigh-Ritz ITerative subspace projection technique

1. Select a proper projection subspace $\mathcal{V}$.

2. Compute a pair (θ, z) to satisfy the Galerkin condition:

$$T(\theta)z \perp \mathcal{V} \quad \text{for} \quad z \in \mathcal{V}.$$

3. Expand or restart the projection subspace $\mathcal{V}$

[Betcke and Voss,'04], [**Voss,'04**], [Mehrmann and H. Voss,'04]

NRRIT – matrix version

1. Select an orthonormal basis Q of the proper subspace $\mathcal{V}$ and inintial approximations (θ^ℓ, v^ℓ)

2. Compute a pair (θ, g) with initials $(\theta^\ell, Q^T v^\ell)$ to satisfy

$$T_Q(\theta)g = 0,$$

where

$$T_Q(\theta) = Q^H T(\theta) Q$$

3. Expand or restart Q

Ritz pairs: (θ, Qg)
Residual: $r = T(\theta)Qg$

Two critical issues:

(a) what are proper initial approximations (and Q) and ordering?

(b) how to expand or restart Q?

Main features of our implementation of NRRIT

- Proper initial approximations and ordering (θ^ℓ, v^ℓ)

- Preserving real symmetry

$$Q = \mathrm{orth}([\, \mathrm{Re}(V) \;\; \mathrm{Im}(V)\,]),$$

The reduced nonlinear eigenvalue problem

$$T_Q(\theta)y = 0,$$

where

$$T_Q(\theta) = Q^T T(\theta)Q = K_Q - \theta M_Q + \mathbf{i} \sum_{j=1}^{p} (\theta - \sigma_j^2)^{\frac{1}{2}} W_{Q,j}$$

with $K_Q = Q^H K Q$, $M_Q = Q^T M Q$ and $W_{Q,j} = Q^T W_j Q$.
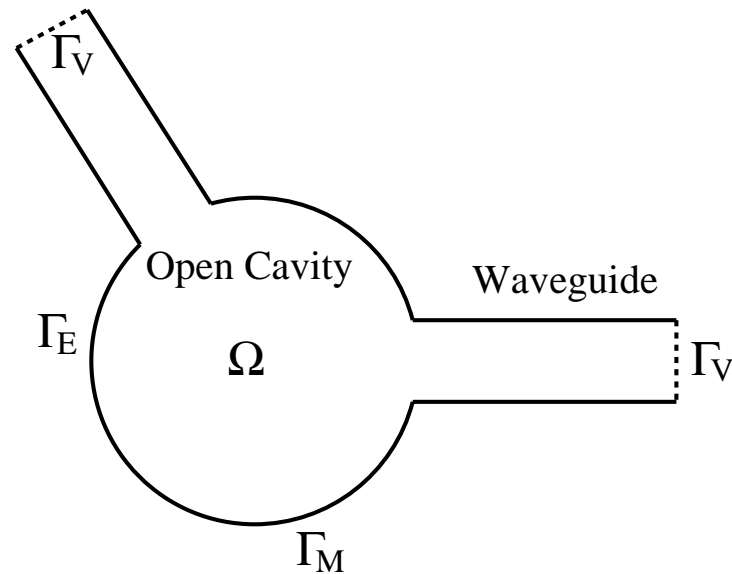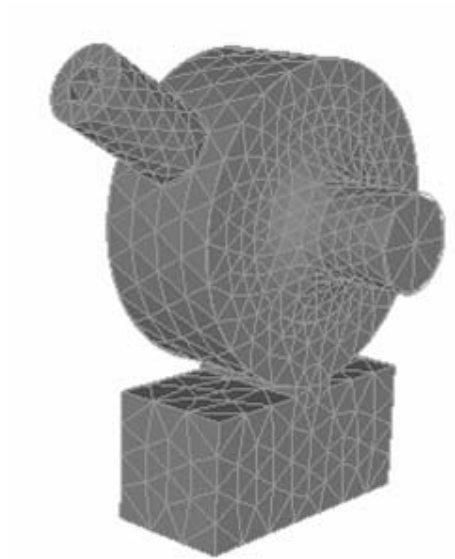
- ...

Example

The NEP with two cutoff values

$$T(\lambda)x = \left[K - \lambda M + \mathbf{i}\sqrt{(\lambda - \sigma_1^2)}W_1 + \mathbf{i}\sqrt{(\lambda - \sigma_2^2)}W_2\right] x = 0,$$

$N = 9956, nnz(K) = nnz(M) = 148,318.\ nnz(W_1) = 57, nnz(W_2) = 293.$

Performance data

Convergence threshold:

$$\frac{\|T(\theta)Qg^\ell\|}{\|T(\theta)\|\,\|Qg^\ell\|} \leq \epsilon \quad \text{for } \ell = 1, 2, \ldots, 10$$

CPU in second:

ϵ	IIT		MSLP		NRRIT	
	Iters	E-Time	Iters	E-Time	Iters	E-Time
10^{-8}	15	71.98	12	79.48	46	22.95
10^{-10}	18	85.92	16	96.19	69	32.91
10^{-12}	22	104.47	20	115.33	87	42.08
10^{-14}	24	113.97	21	120.22	114	57.59

IIT = Inverse ITeration
MSLP = Method of Successive Linear Problem

Ongoing work

- Understanding of NRRIT: subspace expansion, restarting, convergence analysis

- Accuracy of computed eigenvalues (external Q_e-values)

- Verification (missing ones?)

- Software development (Omega3P package)

- Large-scale NEP ($p = 8 \sim 24$, DOFs $= 10^6 \sim 10^7$)