Enabling Technologies for Petascale Electromagnetic Accelerator Simulation*

Community Petascale Project for Accelerator Science and Simulation (COMPASS)

The SciDAC2 Accelerator project at SLAC aims to simulate an entire three-cryomodule RF unit of the International Linear Collider (ILC) main Linac. Petascale computing resources supported by advances in Applied Mathematics and Computer Science and INCITE program are essential to enable such very large-scale electromagnetic accelerator simulations required by the ILC Global Design Effort.

Determining Deformed Shape of ILC Cavities (SLAC, TOPS/UT, LBNL, Columbia, ITAPS/ANL, SNL, LLNL)

- Due to fabrication errors, the real shape of the ILC cavity deviates from the ideal

- Weighted least squares minimization algorithm by fitting shape parameters to measured frequency and field E:

$$\text{minimize } \mathcal{J} = \frac{1}{2}\alpha\,\Delta\lambda^T\Delta\lambda + \frac{1}{2}\beta\sum_{j=1}^{m}\left(\Delta E^j\right)^T\Delta E^j$$

$$\text{subject to} \quad \mathbf{Ke} - \lambda\mathbf{Me} = 0$$

$$\mathbf{e}^T\mathbf{Me} = 1$$

Minimization procedure

- 82 inversion variables used including cell radius, thickness, length and iris radius

- Gauss-Newton with truncated SVD algorithm for the problem

- Converged results fit measured frequencies well
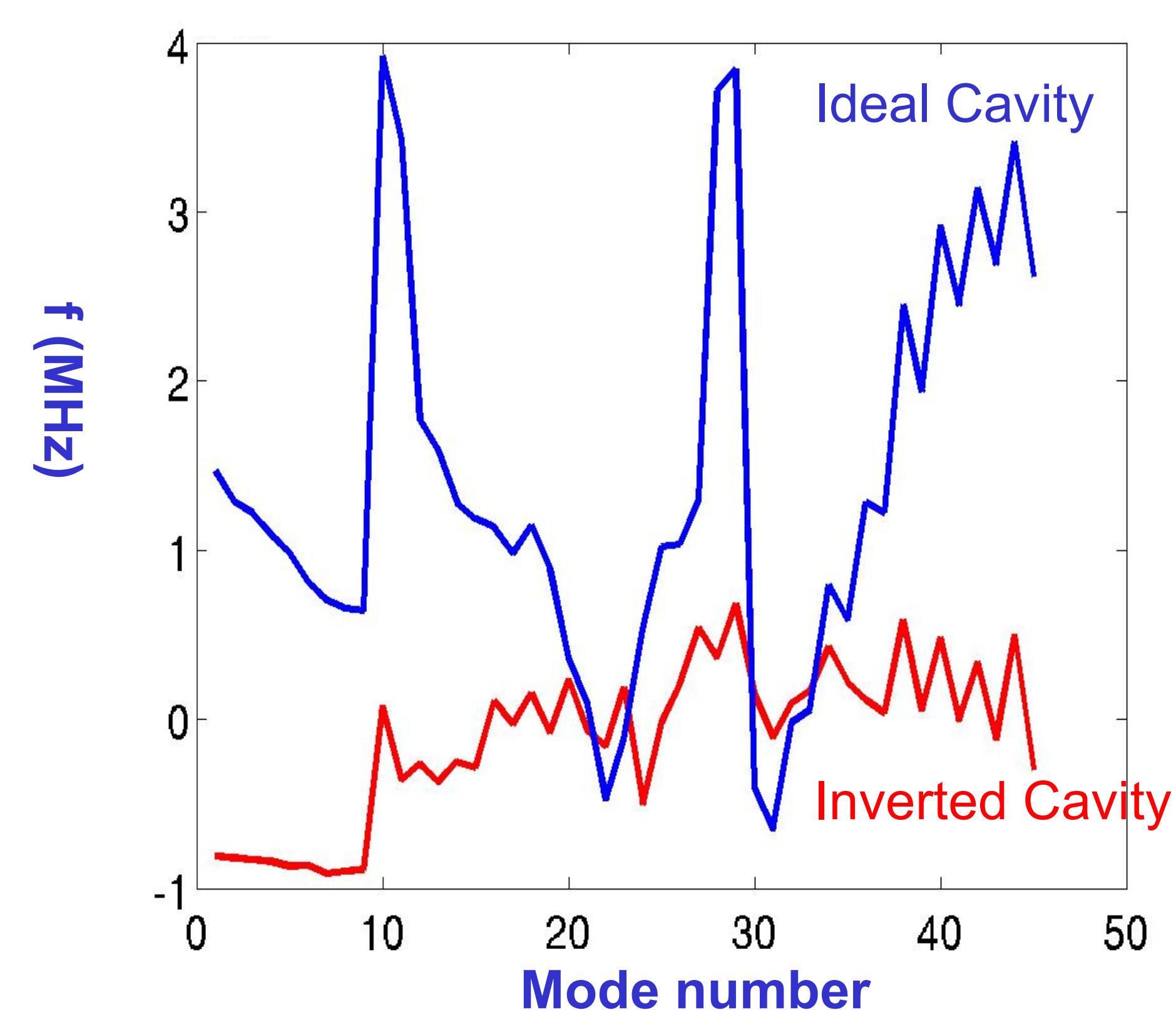
Element Correction for Meshes with Complex Geometries (SLAC, ITAPS/RPI)

- Higher-order curved elements are needed for accuracy
- Mesh generator creates invalidly-curved elements
- Invalid elements lead to inaccurate results and time instabilities
- A mesh correction tool has been developed at RPI to correct invalid tetrahedrons through a set of operations including collapse, split, swap, and shape modifications
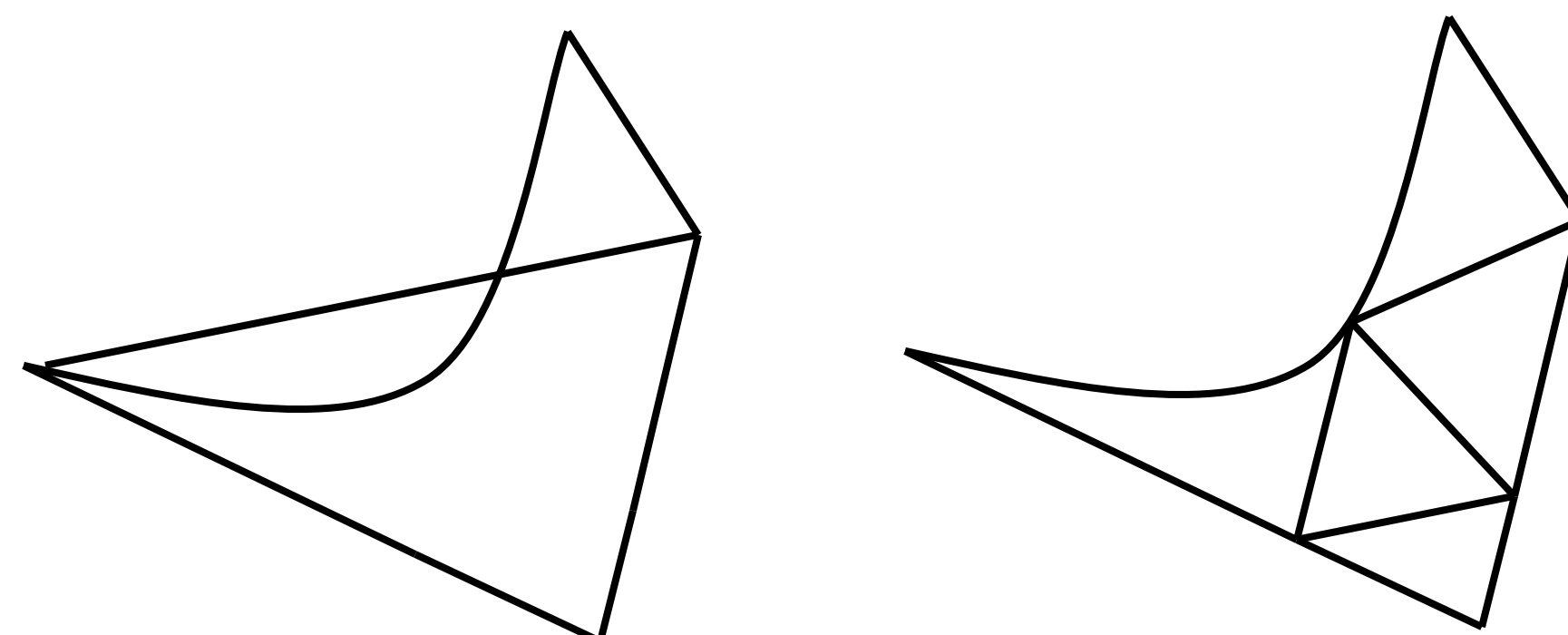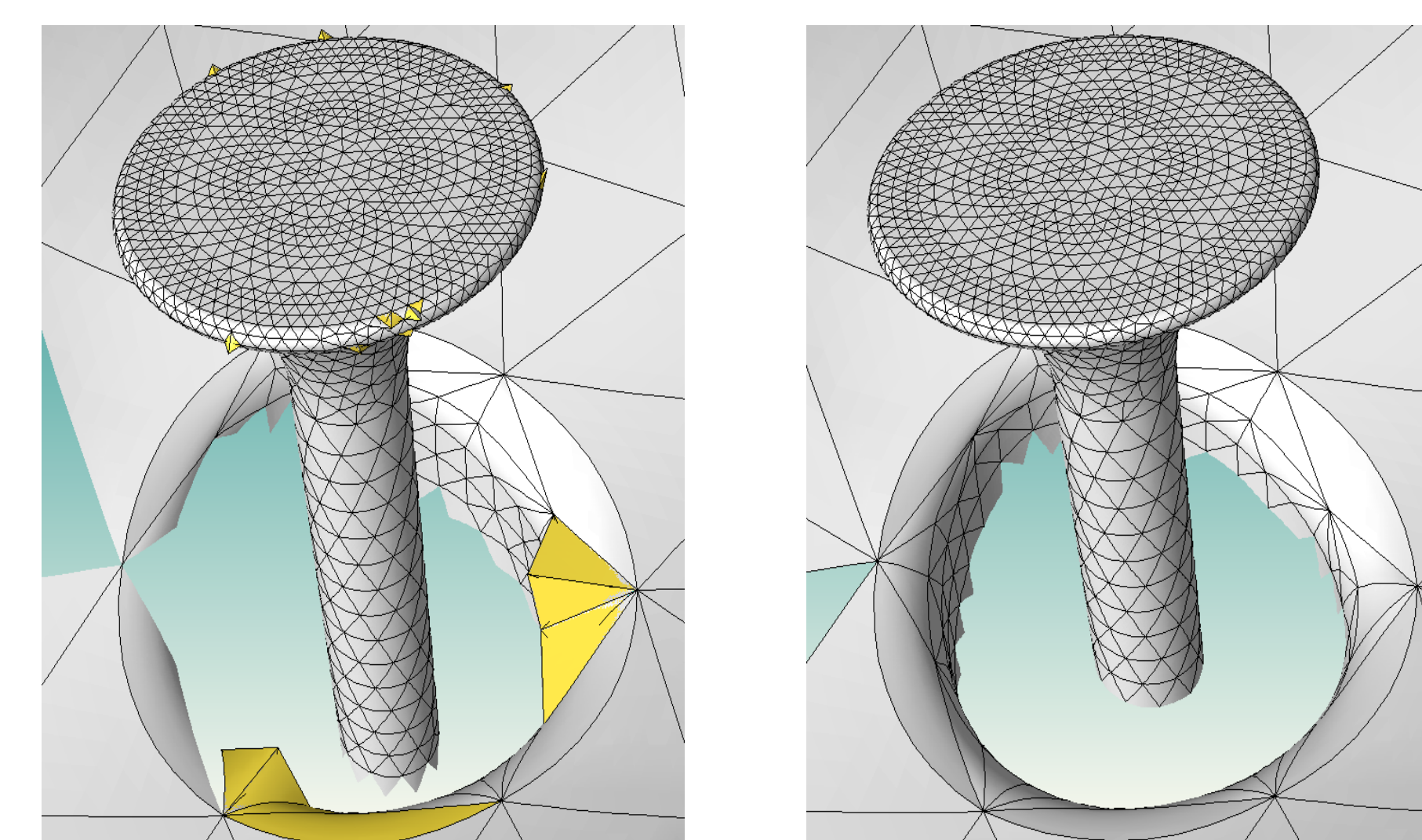
Illustration of Invalid element in 2D and its fix through element split operation

**With corrected mesh, a T3P run is stable and _30% faster_.**

Invalid tetrahedrons (in yellow) inside an accelerator cavity and the corrected mesh

Memory Reduction in Linear Solvers (SLAC, TOPS/LBNL)

- Memory limits the simulation capability even on supercomputers

- Linear solvers with good memory usage scalability needed

- Many methods developed to reduce memory usage

Factorize a Matrix in Single Precision as Precondtioner

$$A\,x = b$$

M (float) b (float)

LDL^T (float) ⟶ x (float)
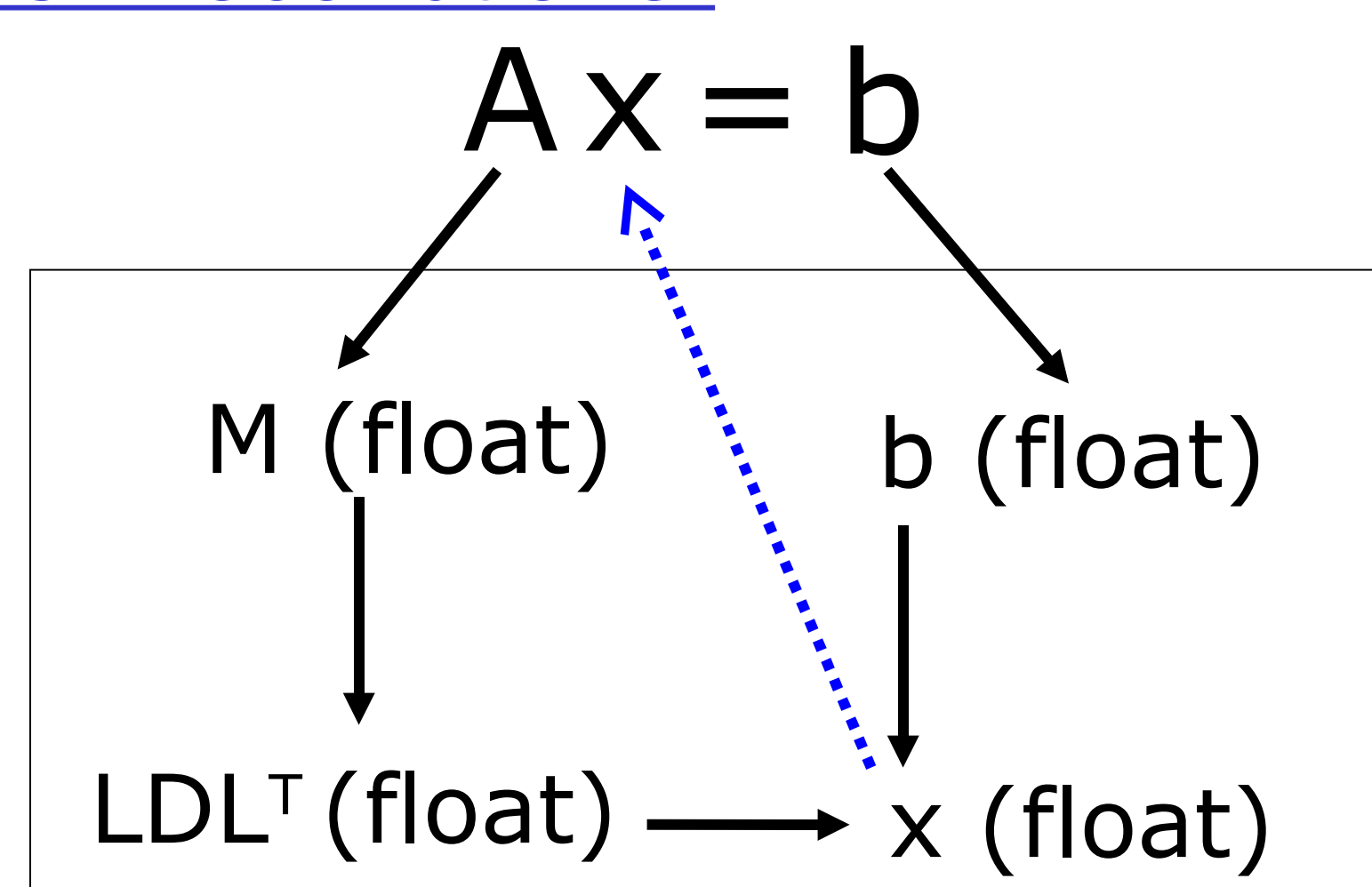
- The method cuts memory usage in half
- Other methods developed, cutting memory usage down to as little as 1/20 at the expense of longer runtime

Method	Memory (GB)	Runtime (s)
MUMPS	155.3	293.3
MUMPS single precision factorization	82.3	450.1

Simulation of ILC 8-cavity Cryomodule, twice as large as the ILC superstructure simulated last year