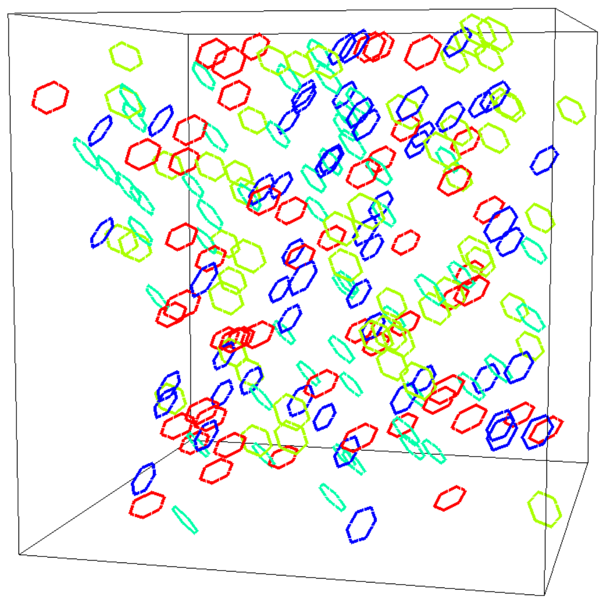
Fast Multipole Methods for Dislocation Dynamics Simulation

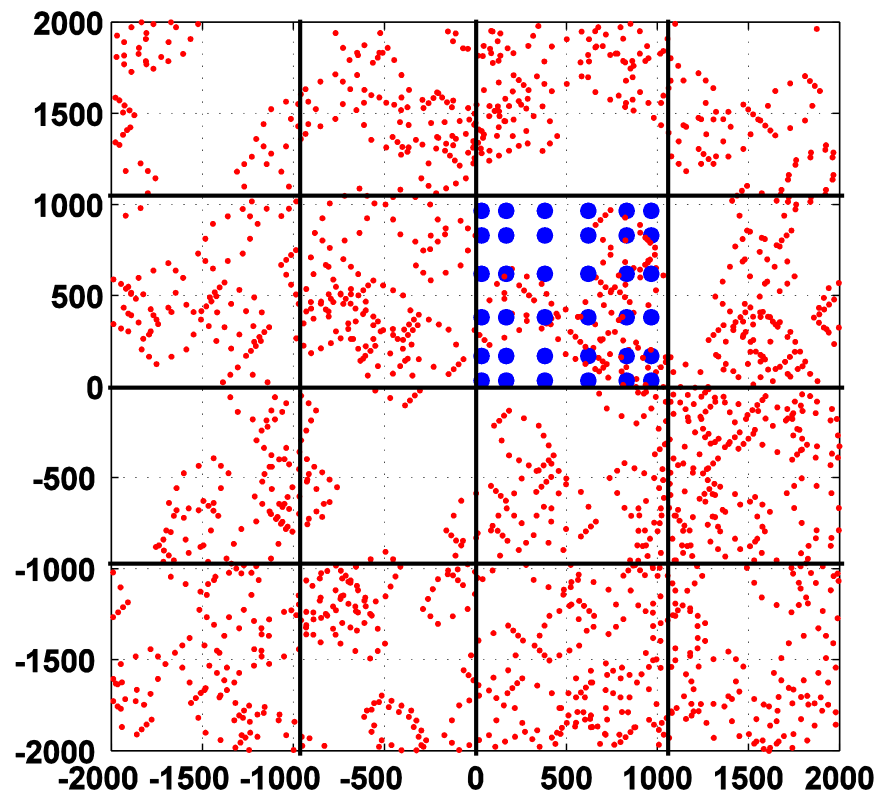
Chao Chen,[1] Sylvie Aubry,[2] Tom Oppelstrup,[2]
Clifton Dudley,[1] Tom Arsenlis,[2] Eric Darve[1]

[1]Stanford University
[2]Lawrence Livermore National Laboratory

Dislocation Interaction

- Problem: It takes $O(N^2)$ flops to evaluate the stress field from N dislocation loops at N points or to compute the interaction force between N loops.





(a) 210 dislocation loops (b) Evaluate stress at Gauss grids in every cell

Isotropic Kernel

- The stress at x from one dislocation loop C with Burger's vector b is given using linear elasticity as

$$\sigma_{\alpha\beta}(\boldsymbol{x}) = \oint_C K_{\alpha\beta wr}(\boldsymbol{R}) b_w dx_r^{'}$$

- Dislocation dynamics simulations often consider isotropic elasticity, where the kernel K is defined with the derivatives of R.

- Different fast multipole methods (FMM) have different advantages.

Anisotropic Kernel

- Extreme environments: high pressure, high temperature or high loading rates.
- Anisotropic kernel is more complicated and is defined using spherical harmonics.

$$\frac{\partial G_{vp}}{\partial x_d}(\boldsymbol{R}) = \frac{1}{R^2} \sum_{q=0}^{\infty} \sum_{m=0}^{2q+1} \Re \left(S_{vpd}^{qm} (\boldsymbol{T} \cdot e_{12})^m (\boldsymbol{T} \cdot e_3)^{2q+1-m} \right)$$

- Currently, rarely used due to computational cost.
- Black-box fast multiple methods are very handy for such kernel.

Fast Multipole Method

- Reduces the cost from $O(N^2)$ to $O(N)$.
- Two ingredients:

  (1) Low rank approximation for far-field interactions.
  (2) Hierarchical decomposition.
- Computing and applying the far-field (M2L) operator is the most expensive step.

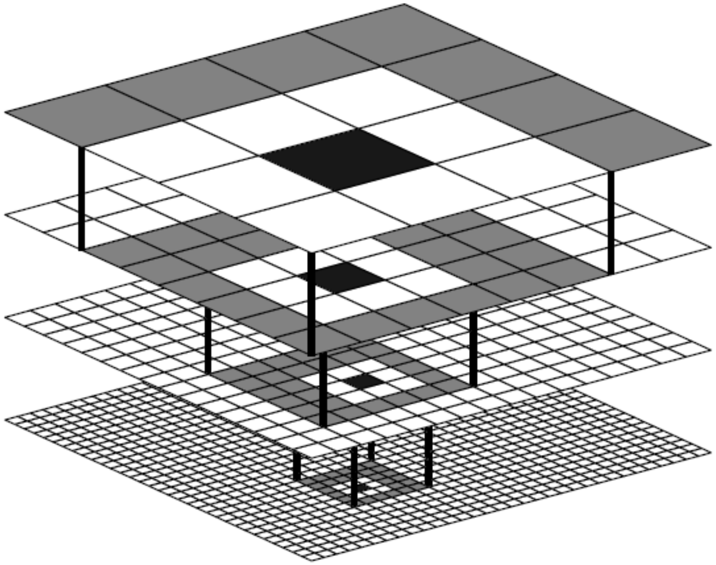
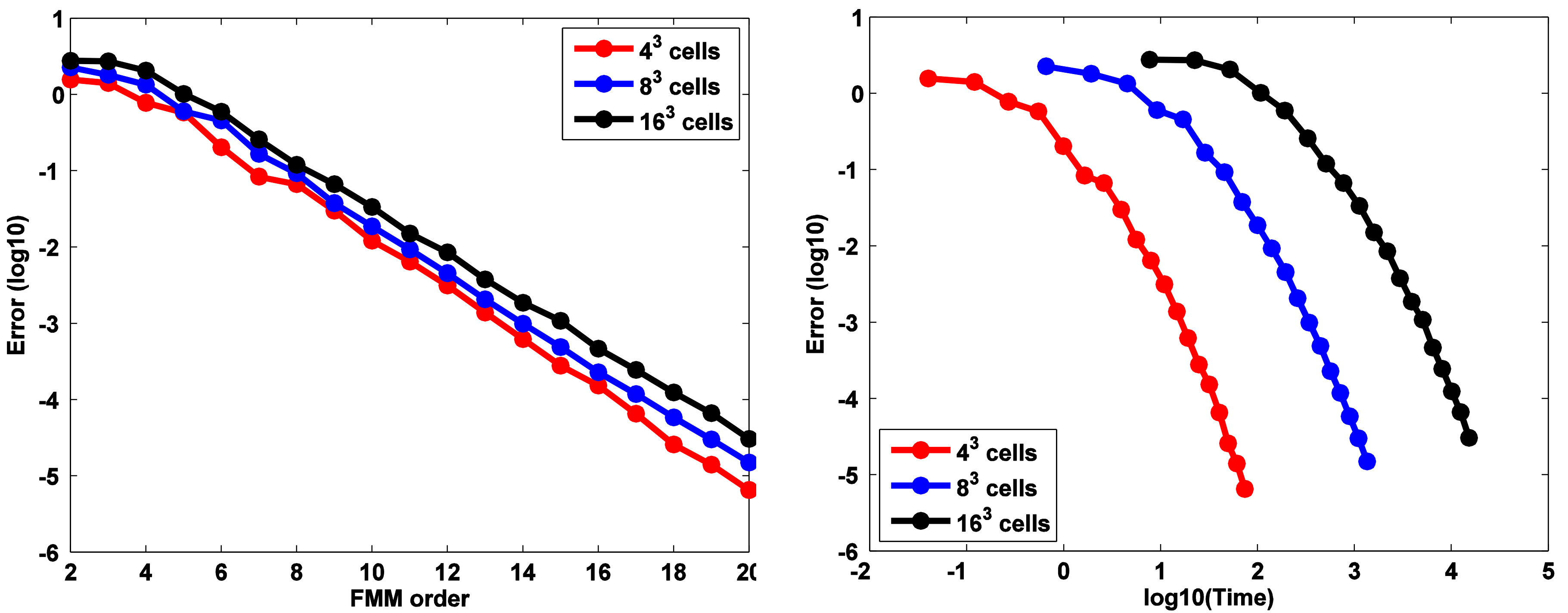


Fig: Recursively divide the domain

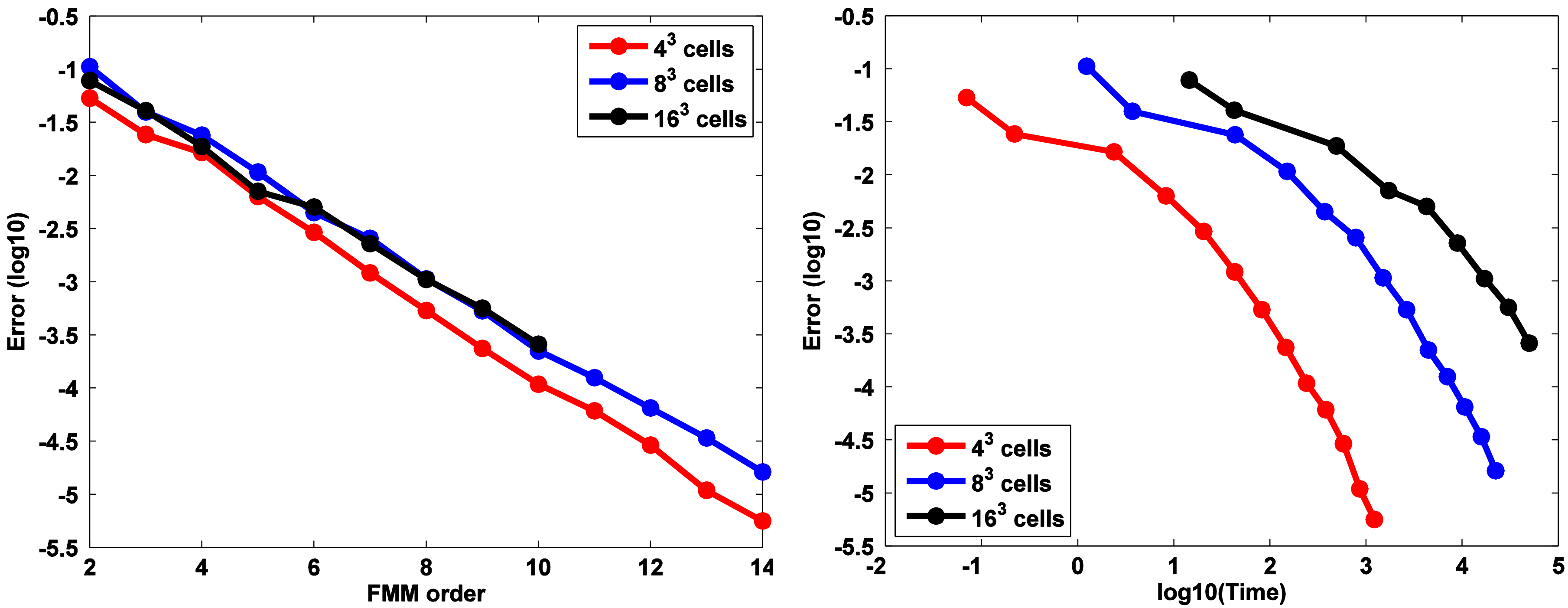
FMM(1): Spherical Harmonics

- Expand the isotropic kernel using spherical harmonics to construct low rank approximation.
- Optimization: tensor symmetry, vanishing terms, recurrence relationship of the integrals.



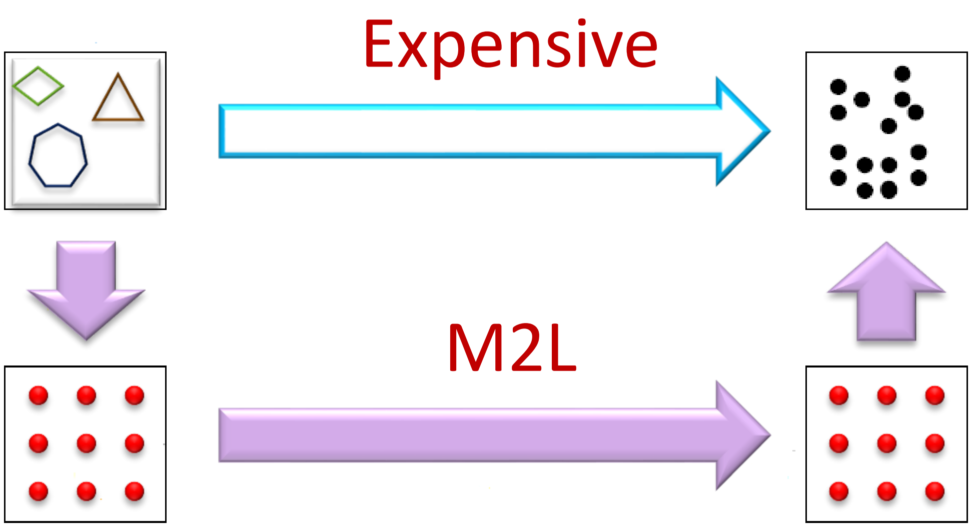
FMM(2): Taylor Series

- Expand the isotropic kernel in Taylor series. This works for any analytical kernel in principle.
- Optimization: considering symmetry, only 13 M2L are computed instead of 189.



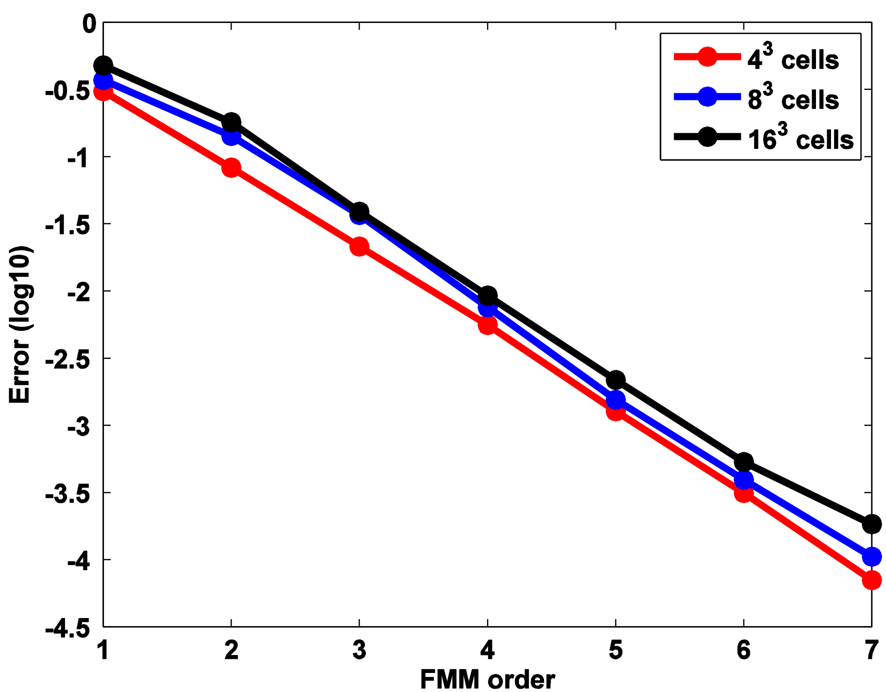
Analytical Interpolation

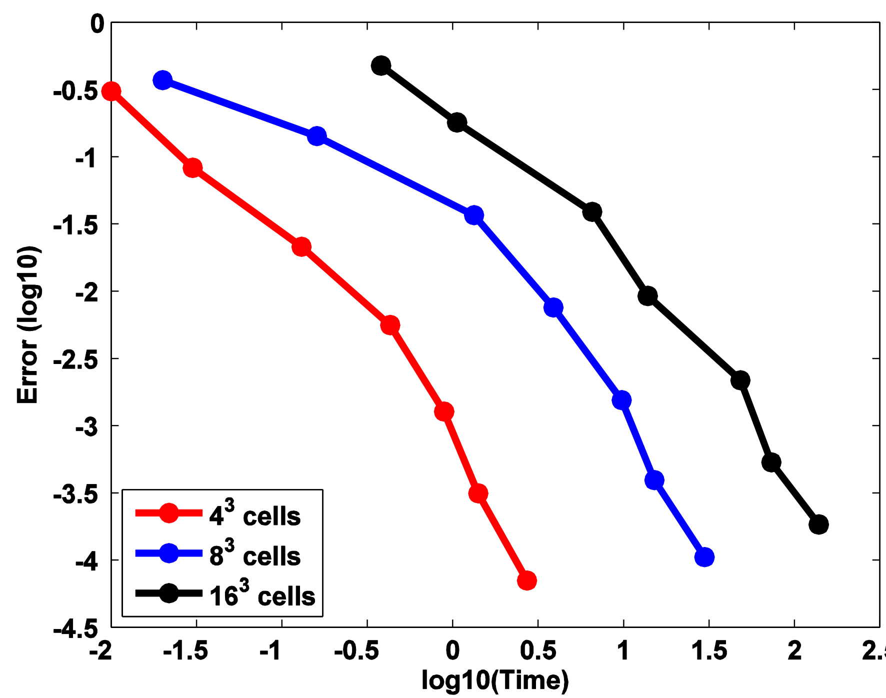
- Approximates the kernel using interpolation. Kernel-independent methods: they only require kernel evaluations.
- Thanks to the (fixed) interpolation grids, M2L can be pre-computed and accelerated.



FMM(3): Chebyshev Interpolation

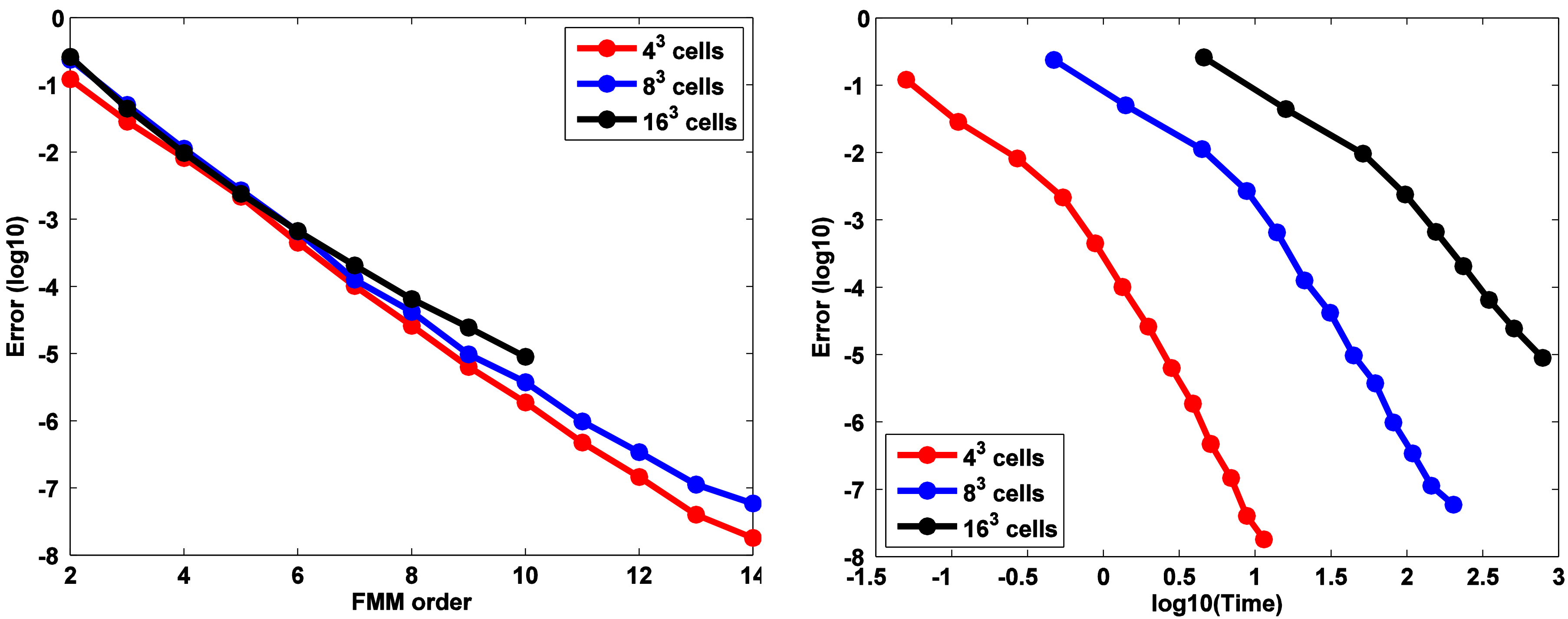
- Interpolation error is optimal in the infinity-norm.
- Use SVD to compress M2L.





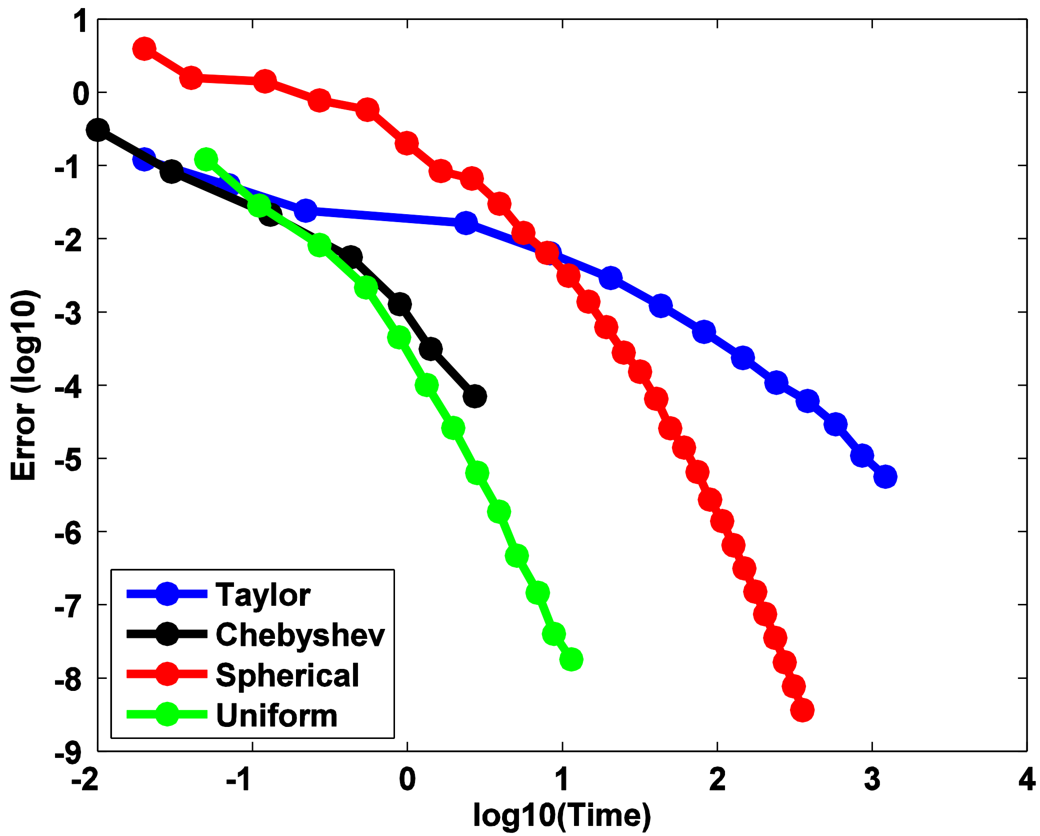
FMM(4): Uniform Interpolation

- M2L storage becomes O(p) while they are O(p^2) in Chebyshev method, where p is the number of grid points.
- M2L is a Toeplitz matrix, which enables use of FFT.



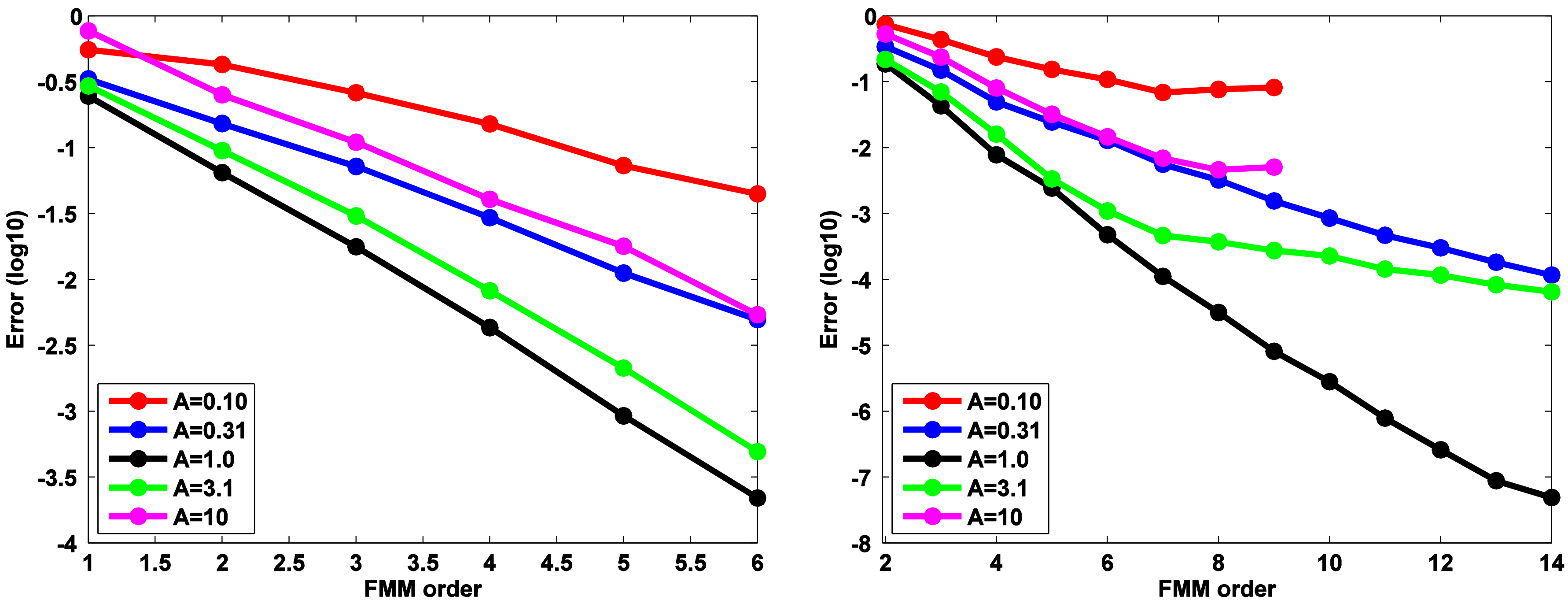
Timing Results for Isotropic Kernel

- Expansion methods are slower.
- Interpolation methods are faster, but suffer from larger storage needs.



Anisotropic Kernel

- Easy for interpolation methods: only need kernel evaluations.
- Hard for expansion methods: requires redo of the math, different implementation and optimization.



(a) Chebyshev interpolation (b) Uniform interpolation

Conclusion

- Expansion methods are specific to the analytical expression.

- Interpolation methods are black box methods that apply to general kernels; work for cases where the kernel is user-defined ("outside" the FMM library), is complicated, or is only known numerically.

- Interpolation methods can be very fast because of pre-computation and acceleration of the M2L operator.