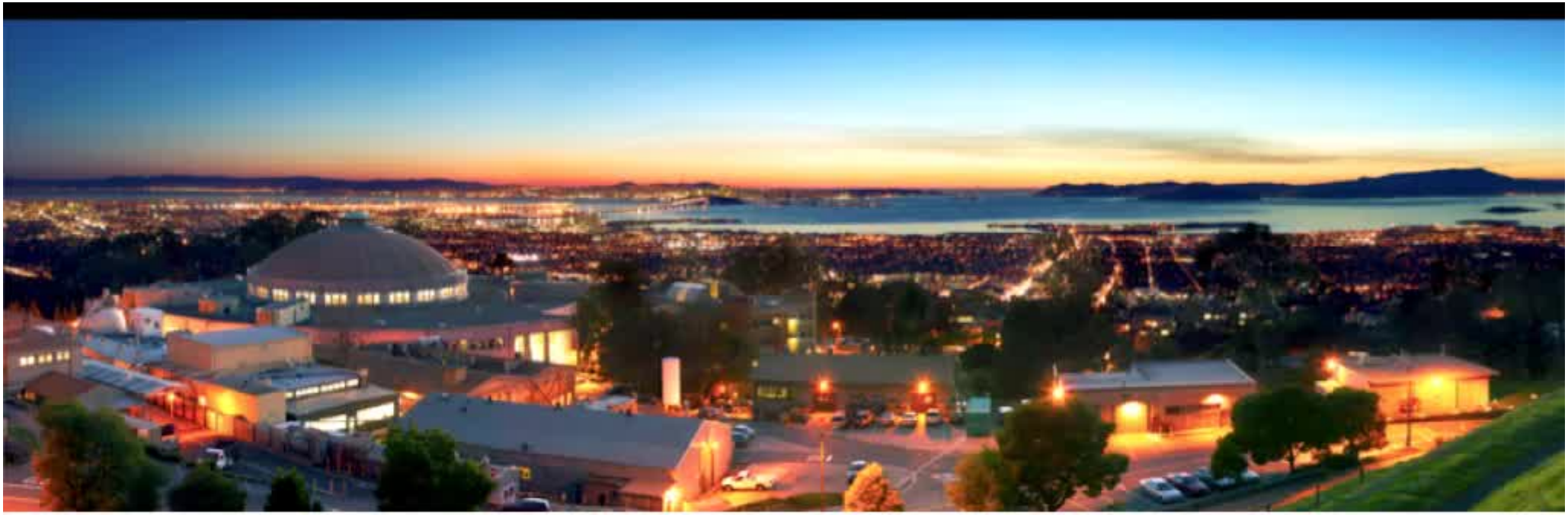

Large-scale Eigenvalue Calculations in Scientific Problems

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BERKELEY LAB

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  - Lin Lin
  - Christopher Haine
  - Chao Yang

- Reference: "Parallel eigenvalue calculation based on multiple shift-invert Lanczos and contour integral based spectral projection method", Parallel Computing, Vol. 40, No. 7 (2014), pp.195-212.

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Large-scale symmetric linear eignvalue problems

- Computing a relatively "large" number of eigenpairs
  - What is "large"?
    - 1% of one million = 10,000
  - Kohn-Sham density functional theory based electronic structure calculation. The number of eigenpairs is proportional to the number of electrons (hundred to thousands to hundreds of thousands depending on the system)
  - Excited state calculation through Green's function formalism of many-body perturbation theory (the GW approximation)

- MS37 (Thursday):
  - Andreas Stathopoulos, "Techniques for Computing a Large Number of Eigenpairs of Sparse, Hermitian Matrices"

Methods for computing many eigenpairs

- LAPACK or ScaLAPACK if the NEV is a significant portion of the matrix dimension (50%, 30% or maybe even 20%) unless the eigenvectors are structured (e.g., block diagonal)
- Compute all at once using block methods
  - LOBPCG
  - Chebyshev-Davidson
  - Block Krylov-Schur
  - ...
- Spectrum slicing
  - Divide the spectrum into subintervals
  - Compute interior eigenvalues within each interval

Why spectrum slicing?

- More concurrency; eigenvalues belonging to different intervals computed (almost) independently

- Reduced Rayleigh-Ritz/orthogonalization cost

Related Talks

- MS37 (Thursday):
  - Yousef Saad, "Spectrum Slicing by Polynomial and Rational Function Filtering"

- MS50 (Friday):
  - Vasilis Kalantzis, "Domain Decomposition Algorithms for Large Hermitian Eigenvalue Problems"
  - Tetsuya Sakurai, "A Contour Integralbased Parallel Eigensolver with Higher Complex Moments"
  - Peter Tang, "On the Orthogonality of Eigenvectors Obtained from Parallel Spectral Projection Methods"
  - Guojian Yin, "A Contour-Integral Based Algorithm for Counting the Eigenvalues Inside a Region in the Complex Plane"

Cost model

- Assumption:
  - Matrix dimension: n
  - $p = c_p n, \quad n_e = c_n n$
  - Uniform eigenvalue distribution
  - Factorization and triangular solution costs: $c_f n^{\alpha_f}, c_s n^{\alpha_s}$
  - Parallel efficiencies: $\eta_f, \eta_s \in (0,1)$
  - q processors per interval ($q = p / (n_e / k)$)
  - Rayleigh-Ritz and orthogonalization costs are negligible
- Wall clock time for computing k eigenpairs per interval:

$$W(k) = \frac{c_f n^{\alpha_f}}{q^{\eta_f}} + \frac{c_s n^{\alpha_s} k}{q^{\eta_s}}$$

$$k_{opt} = \left(\frac{\eta_f c_f}{(1-\eta_s) c_s} \right)^{\frac{1}{\eta_f - \eta_s + 1}} \left(\frac{c_n}{c_p} \right)^{\frac{\eta_f - \eta_s}{\eta_f - \eta_s + 1}} n^{\frac{\alpha_f - \alpha_s}{\eta_f - \eta_s + 1}}$$

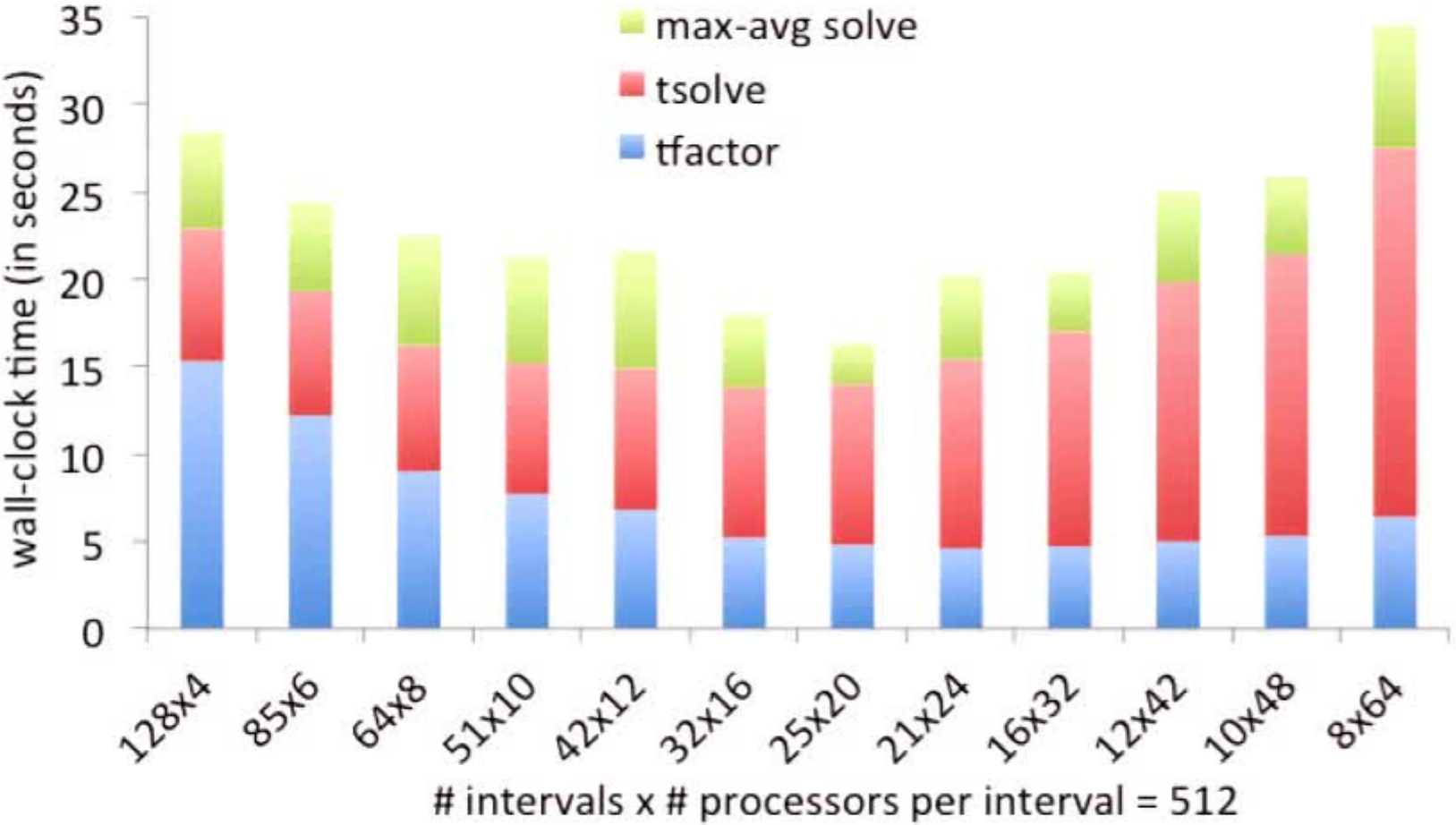
Observations

- When c_n / c_p is constant, optimal k depends on problem size and relative cost of factorization and triangular solution

$$k_{opt} = \left(\frac{\eta_f c_f}{(1-\eta_s)c_s} \right)^{\frac{1}{\eta_f - \eta_s + 1}} \left(\frac{c_n}{c_p} \right)^{\frac{\eta_f - \eta_s}{\eta_f - \eta_s + 1}} n^{\frac{\alpha_f - \alpha_s}{\eta_f - \eta_s + 1}}$$

- When η_f, η_s are close to 1, we should place more eigenvalues in each interval without increasing Rayleigh-Ritz and orthogonalization cost/ slowing down convergence
- When $\eta_f = \eta_s = \eta$
  - $k_{opt} = \left(\frac{\eta c_f}{(1-\eta)c_s} \right) n^{\alpha_f - \alpha_s}$ independent of the total # of processors
  - $W(k_{opt}) = \frac{c_f n^{\alpha_f}}{u} + \frac{\eta}{1-\eta} \frac{c_s n^{\alpha_s}}{u}, \quad u = q^{\eta}$

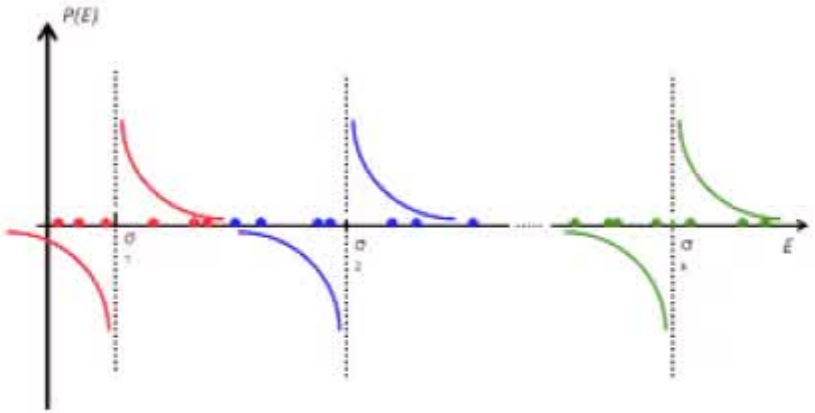
The effect of interval size (MSIL)



Graphene 512

Implementation of multiple shift-invert Lanczos

- Place the target shift in the middle of the interval
- Set *k* to be slight larger than the number of eigenvalues estimated to be in this interval
- Use the implicit restart to limit the size of the Krylov subspace (hence the cost of orthogonalization and Rayleigh-Ritz calculation)
- Set maximum number of restarts to limit the total cost for this interval



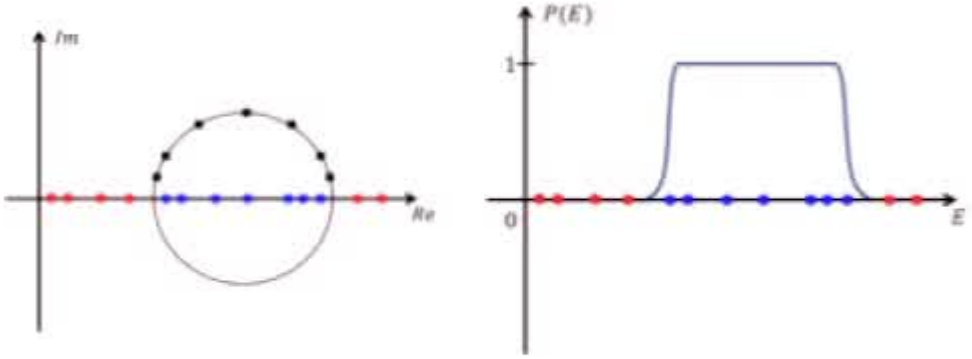
Implementation of contour integral spectral projection method

- Use the FEAST package (Polizzi)
- In most cases, 16 quadrature points (poles) are sufficient for constructing $P = \sum_i (A - z_i I)^{-1} \omega_i$
- Apply the approximate spectral projector P to an orthonormal basis of a subspace S within a subspace iterative (2-3 iterations often sufficient)

Pick an orthonormal basis V for S
While no convergence

- $W \leftarrow PV$
- $V \leftarrow qr(W)$
- Check convergence

- $\dim(S) = 1.5k$



MSIL vs MCISPM

MSIL:

- One factorization per interval
- Real arithmetic
- One solve at a time, a sequential process

MICISPM:

- 8-16 factorizations per interval
- Complex arithmetic
- Multiple right-hand sides.
  - However, if the factor is distributed, the solves cannot be performed completely in parallel
  - Some efficiency (2-3x) can be gained from blocking (BLAS3)

Why is MCIPM less efficient than MSIL on distributed-memory systems?

- Because MCISPM requires multiple complex factorizations, one would like to include as many eigenvalues as possible in an interval to amortize the factorization cost
  - Ideally, the number of eigenvalues should be 8 or 16x those in an MSIL
- But having too many eigenvalues in an interval will increase the cost of triangular substitution
- The number of eigenvalues is also limited by Rayleigh-Ritz/ orthogonalization cost and convergence rate of the subspace iteration

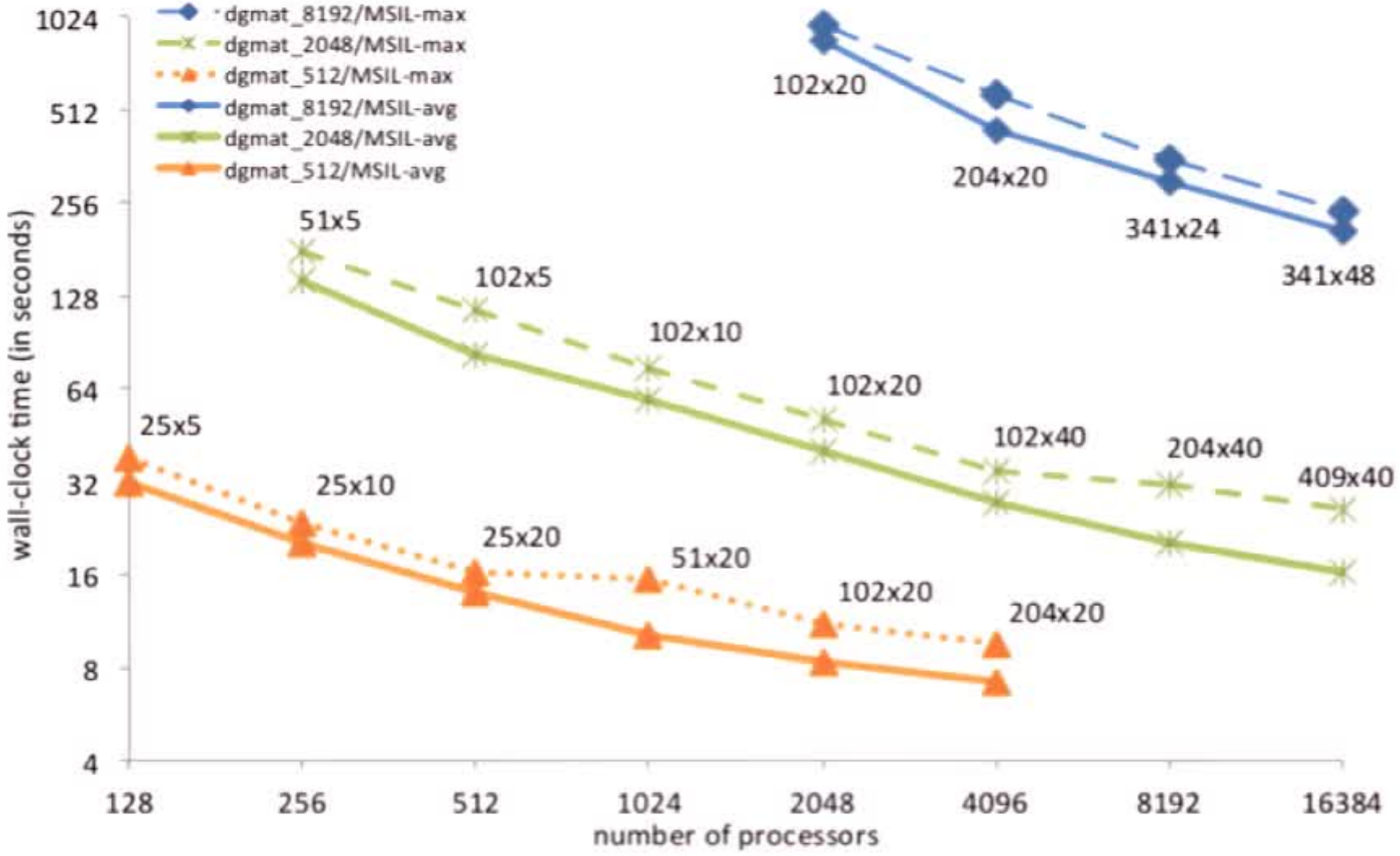
- *The conclusion may be different if each linear system is solved iteratively or if shared-memory parallelism is used*

Weak and strong scaling study

Matrix name	dimension	nnz	L_{nnz}
Graphene128	5120	1M	3.1M
Graphene512	20480	4.1M	43.2M
Graphene2048	81920	16.4M	135.4M
Graphene8192	327680	65.7M	727.5M

- Matrices generated from DGDFT
- Use MUMPS for factorization and triangular solution
- FEAST for MCISPM
- PARPACK for MSIL
- Experiments performed on Hopper at NERSC. Each node has two 12-core AMD Magny Cours 2.1GHz processors, 32GB shared memory
- Convergence tolerance (for relative residual norm) set to 10^{-10}

MSIL strong scaling



MSIL weak scaling

problem	p	$q \times l$	k	t_{wall}	expect/ actual scaling
Graphene512	512	20 x 25	82	16.4	
Graphene2048	2048	20 x 102	80	50.6	3.2/3.1
Graphene8192	8192	20 x 108	96	353	5.2/7

l = # intervals; q = # processors/interval

- The expected scaling factors are calculated from the cost model and the actual time measured for factorization and triangular solutions, and the assumption that $\eta_f = \eta_s = 0.5$

MCISPM Strong scaling

- Graphene2048, n = 81,920, nev = 8,192

p	q x l	k	t_f	t_s	t_{other}	t_{wall}
8,192	256 x 32	256	65	104	37	208
16,384	256 x 64	128	65	52	18	137
32,768	256 x 128	64	65	26	18	104
65,536	256 x 256	32	65	12	27	89
131,072	256 x 512	16	65	6	12	87
262,144	256 x 1024	8	65	3.2	10	83

- Optimal choice of q x l

p	q x l	k	t_f	t_s	t_{other}	t_{wall}
8,192	256 x 32	256	65	104	37	**208**
16,384	512 x 32	256	33	68	30	**131**
32,768	512 x 64	128	33	36	16	**85**
131,072	512 x 256	32	33	9	5	**47**
262,144	1024 x 256	16	24	9	4	**38**

MCISPM weak scaling

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