Numerical Linear Algebra Techniques for Fusion Applications

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Outline

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AORSA

All Orders Spectral Algorithm (AORSA)

- Spectral calculations of wave propagation and heating in tokamak plasmas
- Main developers are Fred Jaeger, Lee Berry, Don Batchelor, David Green at ORNL
- SciDAC-1 fusion project, *Numerical Calculations of Wave-Plasma Interactions in Multi-dimensional Systems*, Don Batchelor as PI
- SciDAC-2 fusion project, *Controlling Fusion Plasmas: Electromagnetic Wave Effects Center for Simulation of Wave-Plasma Interactions (CSWPI)*, Paul Bonoli as PI

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AORSA

- Models the response of plasma to radio-frequency (RF) waves by solving the inhomogeneous wave equation, or Helmholtz equation

$$-\nabla \times \nabla \times \mathbf{E} + \frac{\omega^2}{c^2}\left(\mathbf{E} + \frac{i}{\omega\epsilon_0}\mathbf{J}_P\right) = -i\omega\mu_0\mathbf{J}_{ant}$$

  where $\mathbf{J}_P$ is plasma wave current computed as an integral operator on $\mathbf{E}$ and $\mathbf{J}_{ant}$ is antenna source current
- Assume weakly non-linear, time average distribution function $f_0(v,t)$ evolves slowly as

$$f(\mathbf{x},\mathbf{v},t) = f_0(\mathbf{x},\mathbf{v},t) + f_1(\mathbf{x},\mathbf{v})e^{-i\omega t}$$

  where $f_1(\mathbf{x},\mathbf{v})\exp(-i\omega t)$ evolves on a fast RF time scale
- Fluctuating plasma current $\mathbf{J}_P$ due to wave

$$\mathbf{J}_P(\mathbf{x}) = \int d\mathbf{x}'\sigma(\mathbf{x},\mathbf{x}'-\mathbf{x})\cdot\mathbf{E}(\mathbf{x}')$$

  where $\mathbf{x}$ is position vector, $\sigma(\mathbf{x},\mathbf{x}-\mathbf{x}')$ is the plasma conductivity kernel

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Fourier Harmonics

- The RF electric field is expanded in Fourier harmonics

$$\mathbf{E}(x,y,\varphi) = \sum_{n,m,\ell} \mathbf{E}_{n,m,\ell} e^{i(k_n x + k_m y + \ell\varphi)}$$

  where $x = R - R_0$, $y = Z$, n, m, ℓ are Fourier mode numbers.
- In the limit of a spatially homogeneous plasma

$$\mathbf{J}_P(x,y,\varphi) = \sum_{n,m,\ell} \sigma(k_n, k_m, \ell) \cdot \mathbf{E}_{n,m,\ell} e^{i(k_n x + k_m y + \ell\varphi)}$$

  where $\sigma(k_n, k_m, \ell)$ is the plasma conductivity tensor.
- For tokamak geometry with symmetry about the toroidal axis, the φ harmonics can be uncoupled and calculated separately.

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Linear Equations

- Collocation method on a 2D rectangular grid is used to generate the large (dense) system of linear equations.
- System size $N = 3 * M_x * M_y$ where M_x and M_y are the number of Fourier modes used.
- For $M_x = M_y = 256$, system size N is $196,608$, which requires about 618 GBytes of memory and about $20 * 10^{15}$ flops of computation.
- Problem size $N = 3M^2$, storage scales as $O(N^2)$ or $O(M^4)$ and work scales as $O(N^3)$ or $O(M^6)$.
- Complex*16 system solved using ScaLAPACK LU solver.

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Performance Optimization

- Reduced system size by considering only points inside the plasma.

$$\begin{pmatrix} A_{11} & A_{12} \\ & I \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b1 \\ b2 \end{pmatrix}$$

  where x_1 are variables inside plasma and x_2 are variables outside plasma
- Roughly about $1/3$ of points outside plasma, so solving with $(2/3N)$ requires about $1/3$ amount of time
- Requires formulation in configuration space (not in Fourier space) to identify points outside plasma.
- Require Fourier transform of entire row of matrix and data redistribution for ScaLAPACK

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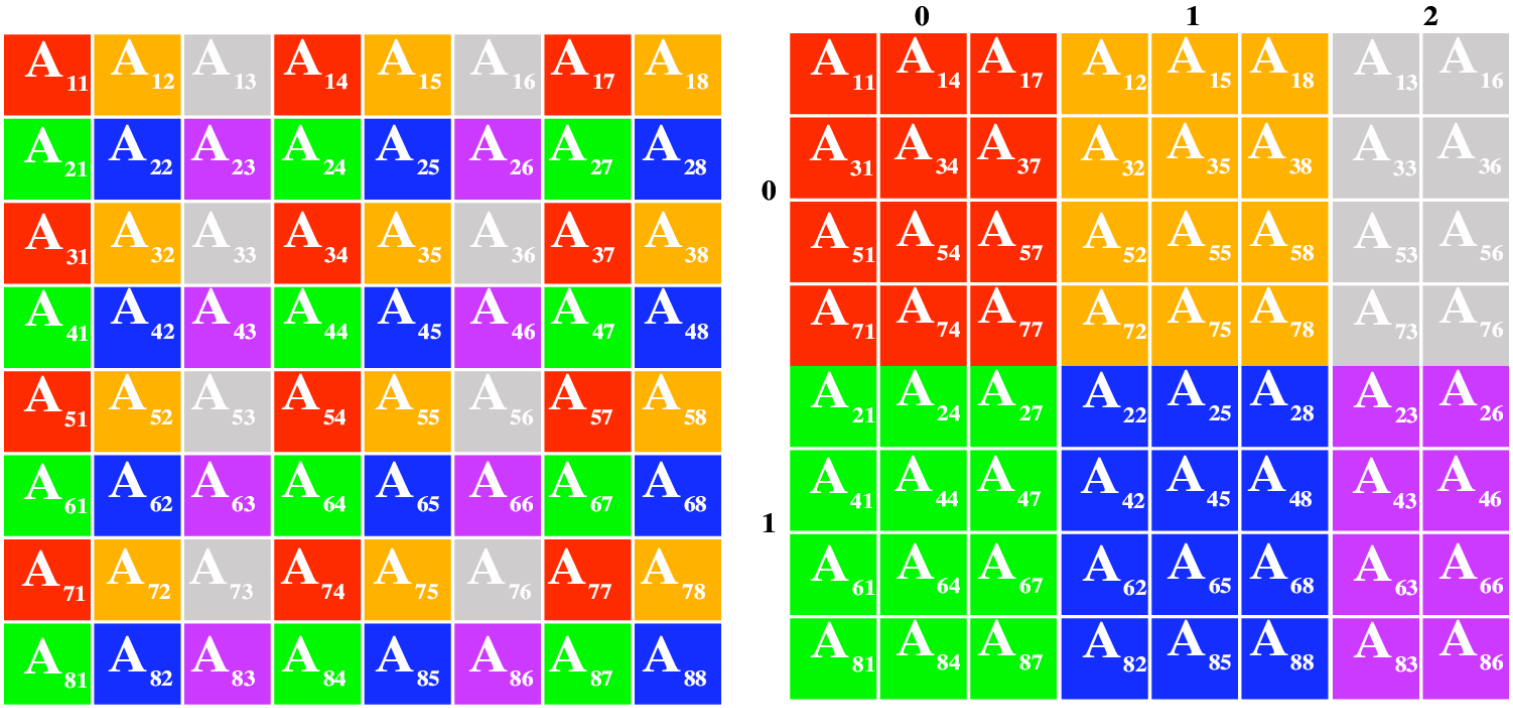
2D Block Cyclic Distribution



Global (left) and distributed (right) views of matrix

Load Imbalance

- Computation in narrow vertical region near mode conversion layer may lead to load imbalance
- Randomize reordering to redistribute work.
- Reuse LU factorization as preconditioner for a range of parameters
- Reduced precision (complex*8) LU factorization with iterative refinement in some cases
- Difficult to find effective preconditioner for iterative method

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High Performance Linpack (HPL) Benchmark

- Reduced scalability and efficiency of ScaLAPACK over 5000 processors
- HPL benchmark used in TOP500 ranking of world's fastest supercomputers
- Solves real*8 dense linear system in 2D block cyclic distribution, rhs is column $(N+1)$
- Multiple options and enhancements with look-ahead to reduce length of critical path, options for performing broadcasts, recursive left-looking or right-looking factorization methods
- Conversion to use complex*16 and complex*8, modify storage layout, return pivot vector, correct pivoting in lower triangular part

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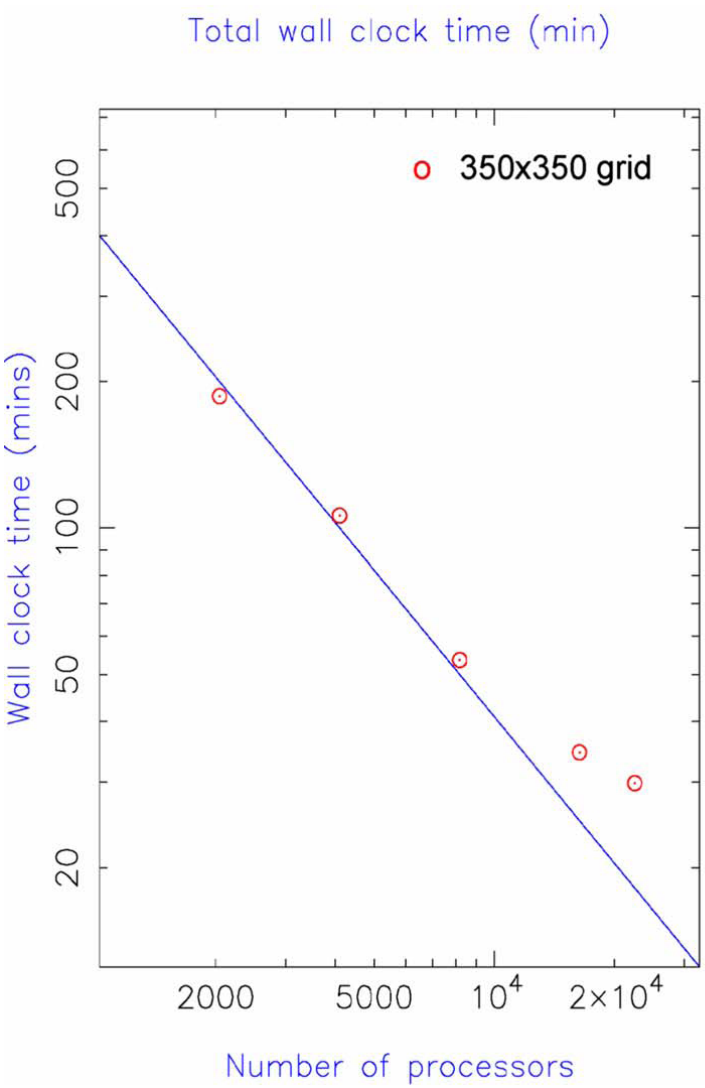
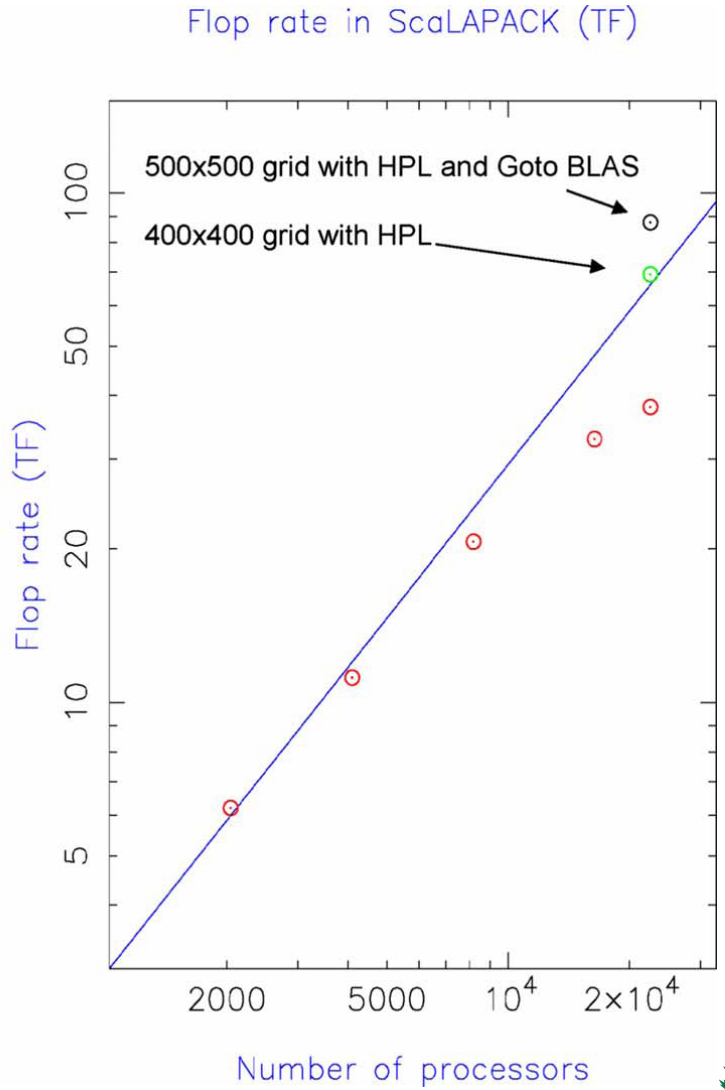
Scalability





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Mixed Precision HPL

- Need storage for extra copy of complex*8 matrix
- Not too ill-conditioned, condition number less than 10^7

Table 1: Run times and Gflop rates per core for complex matrix size of 60,000.

Processor grid	Comple*16 ScaLAPACK LU	Complex*8 ScaLAPACK LU	Complex*8 HPL LU	Mixed precision solver
8×8	1580s (5.7GF)	871s (10.3GF)	732s (12.3GF)	757s
16×16	481s (4.7GF)	280s (8.0GF)	213s (10.6GF)	221s
32×32	185s (3.0GF)	117s (4.8GF)	71s (7.9GF)	76s
64×64	104s (1.4GF)	67s (2.1GF)	30s (4.7GF)	34s
128×128	89s (0.4GF)	51s (0.7GF)	19s (1.9GF)	23s

Run times and Gflop rates per core for complex matrix size of 60,000 (Jaguar XT4)

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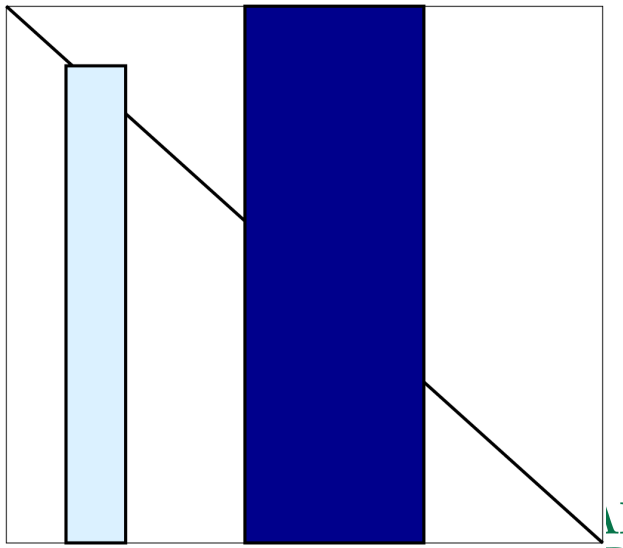
Out-of-core Factorization on GPU

- Bottleneck in data transfer between CPU/GPU
- MAGMA 1.0 limited to matrix in GPU memory
- Out-of-core approach to solve large problems

$$\begin{pmatrix} L_{11} & \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} U_{11} & U_{12} \\ & U_{22} \end{pmatrix} = \begin{pmatrix} A_{11} & A_{21} \\ A_{12} & A_{22} \end{pmatrix}$$

1. Factor diagonal block, $L_{11}U_{11} = A_{11}$
2. Solve for lower triangular part,
   $L_{21}U_{11} = A_{21} \rightarrow L_{21} = A_{21}/U_{11}$
3. Solve for upper triangular part,
   $L_{11}U_{12} = A_{12} \rightarrow U_{12} = L_{11}\ A_{12}$
4. Update and solve for lower part,
   $L_{22}U_{22} = A_{22} - L_{12}U_{21}$



Out-of-core Factorization on GPU

	MKL (12 CPU)	MAGMA 1.0	Out-of-core algorithm
N=25,000	121 Gflops/s	271 Gflops/s	200 Gflops/s
N=35,000	123 Gflops/s	Out of memory	214 Gflops/s

Table: Comparison of MAGMA 1.0 to out-of-core LU factorization (`DGETRF`) using only 1 GBytes out of 5 GBytes of Nvidia M2070.

	MKL (12 CPU)	MAGMA 1.0	Out-of-core algorithm
N=25,000	122 GFlops/s	266 GFlops/s	246 GFlops/s
N=35,000	123 GFlops/s	Out of memory	263 GFlops/s

Table: Comparison of MAGMA 1.0 to out-of-core Cholesky factorization (`DPOTRF`) using only 1 GBytes out of 5 GBytes of Nvidia M2070.

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Parallel Out-of-core Matrix Factorization on GPU

- Parallel out-of-core complex*16 LU factorization on 15 nodes of GPU cluster.
- Each node has 12 cores (AMD 2.6 GHz) and two Nvidia M2050 GPU (only 1 used).
- Each M2050 GPU has 4.3 GBytes of device memory.
- Computation used 180 MPI tasks (one MPI task per core).
- Narrow panel factored using ScaLAPACK on CPU.
- Parallel BLAS was used for communication.
- Communication requires moving data between CPU/GPU since MPI has access to only CPU memory.

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		ScaLAPACK	Out-of-Core
MB	processor grid	GFLOPs	GFLOPs
64	12×15	1103	1813
128	12×15	1104	1633
64	15×12	1043	1714
128	15×12	885	1554

Table: Comparison of the performance of ScaLAPACK `PZGETRF` with an out-of-core factorization method implemented on both the CPU and GPU for $N = 90,000$ on 180 MPI processes.

Anti-aliasing in AORSA

- *Anti-alias filter in AORSA for modeling ICRF heating of DT plasmas in ITER* by Lee Berry, Don Batchelor, Fred Jaeger, and RF SciDAC Team, presented at 53rd Annual Meeting of the APS Division of Plasma Physics Salt Lake City, Utah, November 14-18, 2011
- Aliasing is a distortion caused in analog-to-digital conversion by a too low rate of data sampling.
- TORIC eliminates aliasing by "over-sampling" in the evaluation of convolutions where the σ is evaluated for twice as many modes as required by the solution

$$\begin{aligned}\mathbf{J}_P(\rho,\vartheta) &= \sum_m \left[\sum_n \sigma^n_{m-n}(\rho)\cdot\mathbf{E}_n\right] e^{im\vartheta} \\ &= \sum_m \mathbf{J}_m e^{im\vartheta}, \quad \mathbf{J}_m = \sum_n \sigma^n_{m-n}(\rho)\cdot\mathbf{E}_n\end{aligned}$$

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Antialiasing in AORSA

- AORSA uses collocation

$$\mathbf{J}_P(x_\ell) = \sum_{j=-N}^{N} \sigma(x_\ell, k_j) \cdot \mathbf{E}_{k_j} e^{ik_j x_\ell} \ ,$$

  where ℓ denotes the spatial point (matrix row), and j denotes the mode number (matrix column).

- Fourier transform of the columns of this matrix, the m-th component of $\mathbf{J}$ looks like

$$\mathbf{J}_m = \sum_{n=-N}^{N} \sigma(k_n - k_m, k_n) \cdot \mathbf{E}_{k_n},$$

  which is similar to the convolution in TORIC.

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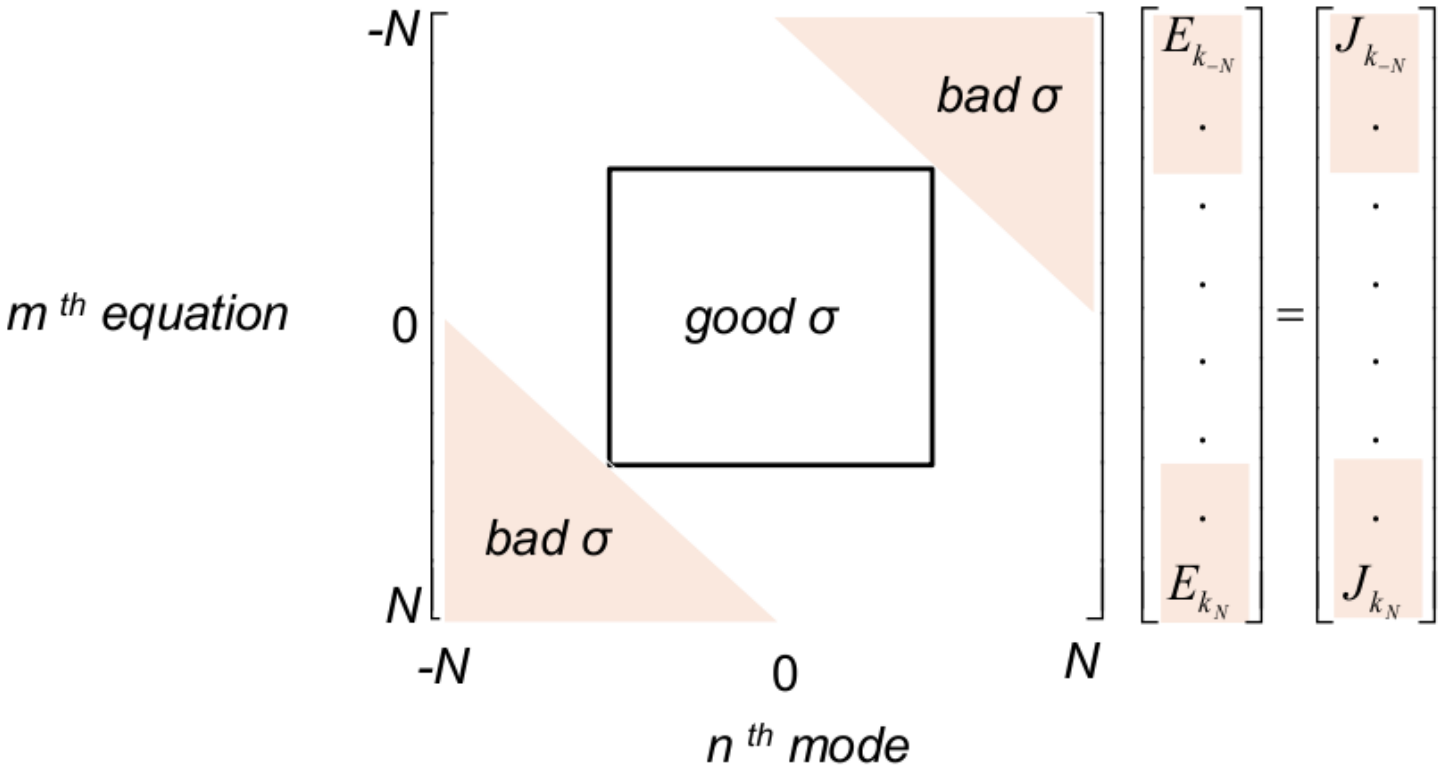
AORSA Matrix Viewed in Fourier Space

There are "bad" regions in the matrix where the σ's are aliased

$$\mathbf{J}_m = \sum_{n=-N}^{N} \sigma(k_n - k_m, k_n) \cdot \mathbf{E}_{k_n},$$



De-aliasing by over-samples on fine grid, an filtering modes

- Fourier transform columns of the large matrix
- Reduce the matrix size by eliminating extra rows and columns that have "bad σ's"
- Fourier transform back to configuration space
- Apply boundary conditions in configuration space for the small problem
- Solve this small "de-aliased" matrix.
- In 2D, it is more difficult and currently solving the large matrix and eliminating the high modes from the solution (very expensive)
- Working on generating and solving the small de-aliased matrix directly rather than solving a larger problem and throwing out half of the solution.

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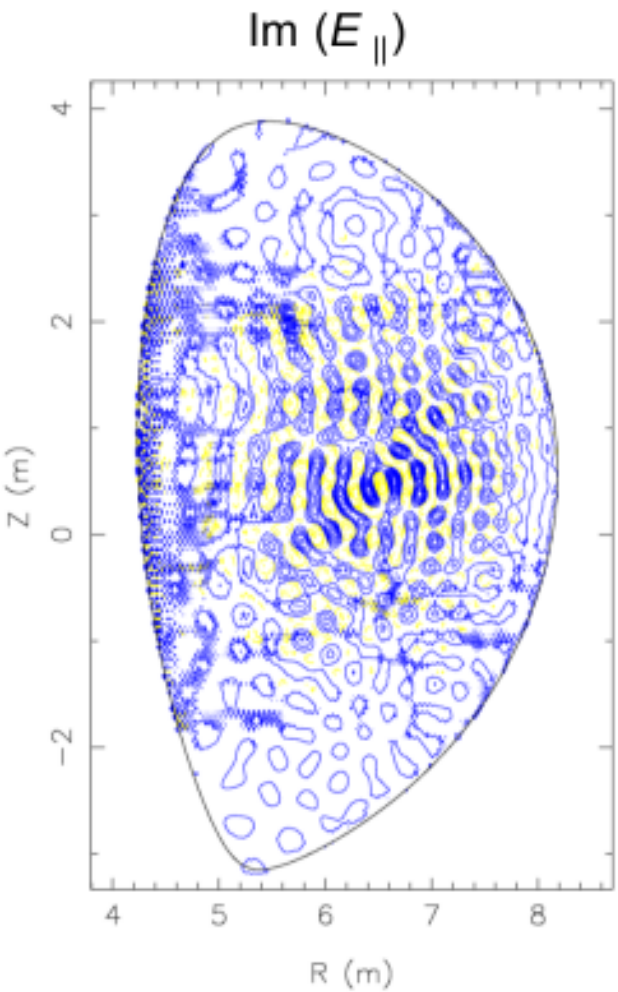
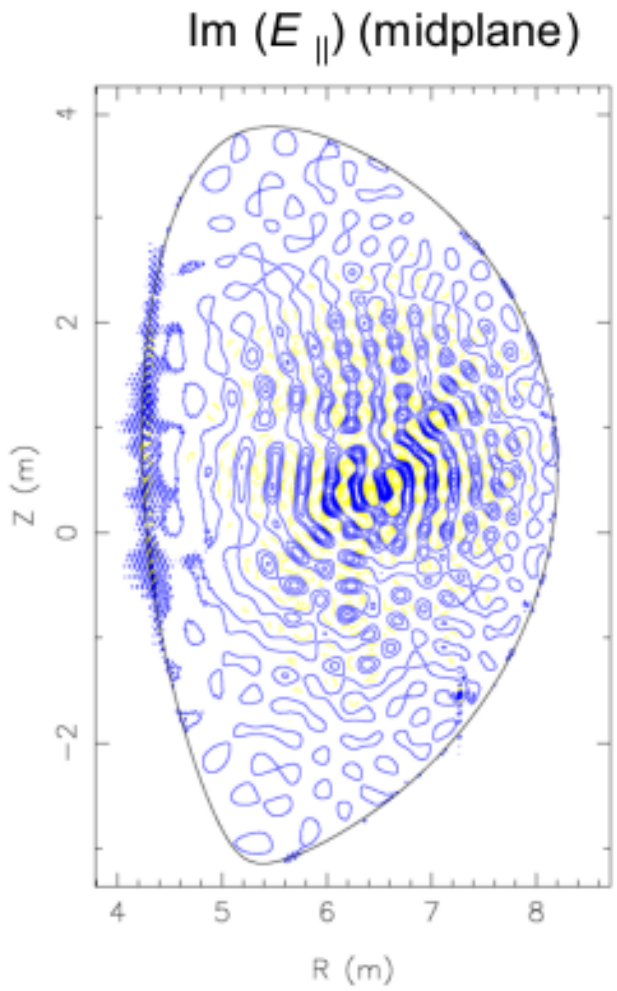
200 modes vs 400 modes with de-aliasing

Short wavelengths close to the edge are better resolved and noise is eliminated.

200x200 (all modes)



400x400 (de-alias 1/2 rule)



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Anderson Acceleration

Anderson Acceleration

- Acceleration of fixed point iteration $x_{k+1} = g(x_k)$ for solving mildly non-linear problem, $f(x) = x - g(x) = 0$
- Rediscovered under different names, also known as vector extrapolation, vector ε-algorithm or Anderson mixing in electronic structure computations
- Iteration to self-consistent solution, e.g. AORSA computes global wave solution and velocity distributions, which is passed to CQL3D Fokker-Planck code to compute quasi-linear diffusion coefficients, which are passed back to AORSA and iterate until self-consistency between wave electric field and resonant ion distribution function
- Idea: find weights α_i such that $1 = \sum_i^k \alpha_i$, $\| \sum_i^k \alpha_i f(x_i) \|$ is minimized, then accelerated solution is a weighted combination of previous solutions $x^* = \sum_i^k \alpha_i x_i$
- The method is simple to implement, and does not require Jacobian information

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Anderson Acceleration

- If $g(x)$ is linearized as $g(x) = J * x + b$ then the method is equivalent to applying GMRES to $(I - J)x = b$
- Note that GMRES finds x_k in Krylov subspace (Span$(b, Ab, A^2b, \ldots, A^k)$) that minimizes the residual $\|b - Ax_k\|_2$.
- The acceleration is restarted after k iterations since computing weights α_i become more ill-conditioned
- D. G. Anderson, *Iterative procedures for nonlinear integral equations*, J. Assoc. Comput. Machinery, 12 (1965), 547-560
- Avram Sidi, *Methods for Acceleration of Convergence (Extrapolation) of Vector Sequences*. Wiley Encyclopedia of Computer Science and Engineering 2008

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Kronecker Products

Kronecker Products

- Kronecker products commonly arise from variable separable formulation, e.g. $f(r,z) = g(r)h(z)$ or approximation on logically rectangular or tensor product grids.
- Let matrix A be $mA \times nA$ and B be $mB \times nB$. For convenience, let them be indexed as $A(ia, ja)$ and $B(ib, jb)$. Let $C = A \otimes B$ (or kron(A, B) in MATLAB notation), then matrix C is size $(mA * mB) \times (nA * nB)$. If matrix A is 3×3, then

$$C = \begin{bmatrix} a_{11}B & a_{12}B & a_{13}B \\ a_{21}B & a_{22}B & a_{23}B \\ a_{31}B & a_{32}B & a_{33}B \end{bmatrix}$$

- Matrix C can be interpreted as a 4-index array $C([ib, ia], [\mathbf{jb}, \mathbf{ja}]) = A(ia, \mathbf{ja}) * B(ib, \mathbf{jb})$, where the composite index $[ib, ia] = ib + (ia - 1) * mB$ is the index in Fortran column-wise order.

Kronecker Product

- Matrix-vector multiply $Y = (A \otimes B) * X$ can be written as very efficient matrix-matrix operations[1],

$$\begin{aligned} Y([ib, ia]) &= C([ib, ia], [\mathbf{jb}, \mathbf{ja}]) * X([\mathbf{jb}, \mathbf{ja}]) \\ &= A(ia, \mathbf{ja}) * B(ib, \mathbf{jb}) * X([\mathbf{jb}, \mathbf{ja}]) \\ &= \boxed{B(ib, \mathbf{jb}) * X(\mathbf{jb}, \mathbf{ja})} * A(ia, \mathbf{ja}) \\ Y &= (B * X) * A^t \end{aligned}$$

- If A and B are $N \times N$, then $C = A \otimes B$ is $N^2 \times N^2$. Kronecker product reduces the work of computing $Y = C * X = (B * X) * A^t$ from $O(N^4)$ to $O(2N^3)$.
- If A and B are sparse matrices, then work is $O(nnz(X)(nnz(A) + nnz(B))$.

[1] We blur the distinction between the matrix $X(jb, ja)$ and vector $X([jb, ja])$ with composite index.

Coding Y = kron(A,B)*X

- Deeply nested loops

```
do ja=1,nA
do jb=1,nB
do ia=1,mA
do ib=1,mB
!   recall C([ib,ia],[jb,ja]) = A(ia,ja)*B(ib,jb)
!  Y([ib,ia]) = C([ib,ia], [jb,ja]) * X([jb,ja])
!
    Y(ib,ia) += B(ib,jb) * X(jb,ja) * A(ia,ja)
enddo; enddo; enddo; enddo
```

- Use array `Z(ib,ja)` to hold common sum over `jb` loop

```
Z(1:mB,1:nA)=matmul(B(1:mB,1:nB),X(1:nB,1:nA))
Y(1:mB,1:mA)=matmul(Z,transpose(A(1:mA,1:nA)))
```

Properties of Kronecker Products

- Other interesting properties of Kronecker products are summarised below,

$$(A + B) \otimes E = A \otimes E + B \otimes E$$
$$(A \otimes B) \otimes E = A \otimes (B \otimes E)$$
$$(A \otimes B)^t = (A^t \otimes B^t)$$

- Reduction of work from $O(N^6)$ to $O(N^3)$.

$$(A \otimes B) * (E \otimes F) = (A * E) \otimes (B * F)$$
$$\mathrm{eig}(A \otimes B) = \mathrm{eig}(A) \otimes \mathrm{eig}(B)$$
$$\det(A \otimes B) = \det(A)^n \det(B)^m, \quad \text{where } A \text{ is } m \times m,\ B \text{ is } n \times n.$$
$$(A \otimes B)^{-1} = (A^{-1} \otimes B^{-1})$$

- If $N = 1000$, $N^6 = 10^{18}$ requires petascale computing, whereas $N^3 = 10^9$ can be performed in seconds on a desktop computer.

1D Interpolation

- Approximate function $f(x) \approx \sum_{j=1}^{n} c_j \phi_j(x)$.
- Basis function $\phi_j(x)$ may be Chebyshev polynomials, B-splines, wavelets or Fourier basis.
- Interpolation condition of tabulated values is used to find c_j's, $f(x_i) = \sum_{j=1}^{n} c_j \phi_j(x_i)$.
- Coefficient c_j's are obtained by solving the linear system $[f(x_i)] = T_x * [c_j]$.
- Note T_x may be sparse if $\{\phi_j(x)\}$ have compact support

$$T_x = \begin{pmatrix} \phi_1(x_1) & \cdots & \phi_n(x_1) \\ \vdots & \ddots & \vdots \\ \phi_1(x_n) & \cdots & \phi_n(x_n) \end{pmatrix} .$$

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1D Interpolation

- Evaluation at new set of points $[f(\tilde{x}_i)]$ is computed as matrix multiply, $[f(\tilde{x}_i)] = T_{\tilde{x}} * [c_j]$,

$$T_{\tilde{x}} = \begin{pmatrix} \phi_1(\tilde{x}_1) & \cdots & \phi_n(\tilde{x}_1) \\ \vdots & \ddots & \vdots \\ \phi_1(\tilde{x}_m) & \cdots & \phi_n(\tilde{x}_m) \end{pmatrix} .$$

2D Interpolation

- Tabulated values $f(x_i, y_j)$ on a rectangular grid is approximated as $f(x,y) \approx \sum_{k,\ell} c_{k\ell}\phi_k(x)\phi_\ell(y)$ (variable separable).
- Interpolation conditions lead to

$$\begin{aligned} \mathrm{vec}(F) &= (T_y \otimes T_x)\,\mathrm{vec}(C) \\ \mathrm{vec}(C) &= \left(T_y^{-1} \otimes T_x^{-1}\right)\mathrm{vec}(F) \\ C &= T_x^{-1} F T_y^{-t} \ , \end{aligned}$$

  where $F = [f(x_i, y_j)]$ $C = [c_{k\ell}]$.
- Evaluation at new points $(\tilde{x}_i, \tilde{y}_j)$ is computed as

$$\left[\tilde{F}_{ij}\right] = (T_{\tilde{y}} \otimes T_{\tilde{x}})\,[c_{k\ell}] = T_{\tilde{x}} C {T_{\tilde{y}}}^t \ .$$

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Higher Dimensions

- Interpolate tabulated values of 4-index function on rectangular (tensor product) grid,

$$f(w,x,y,z) \approx \sum_{ijk\ell} c_{ijk\ell}\phi_i(w)\phi_j(x)\phi_k(y)\phi_\ell(z) \ .$$

- Coefficients computed efficiently as

$$\begin{aligned} \mathrm{vec}(F) &= (T_z \otimes T_y \otimes T_x \otimes T_w)\,\mathrm{vec}(C) \\ \mathrm{vec}(C) &= \left(T_z^{-1} \otimes T_y^{-1} \otimes T_x^{-1} \otimes T_w^{-1}\right)\mathrm{vec}(F) \ . \end{aligned}$$

- Evaluation at new points is computed as

$$\mathrm{vec}(\tilde{F}) = \left(T_{\tilde{z}} \otimes T_{\tilde{y}} \otimes T_{\tilde{x}} \otimes T_{\tilde{w}}\right)\mathrm{vec}(C) \ .$$

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Nearest Kronecker Product

- Given $mn \times mn$ matrix C, find $m \times m$ matrices A, $n \times n$ matrix B to minimise $\|C - A \otimes B\|_F$.
- Let matrix $\tilde{C}$ be a rearrangement of entries of matrix C

$$\tilde{C}([ia, \mathbf{ja}], [ib, \mathbf{jb}]) = C([ib, ia], [\mathbf{jb}, \mathbf{ja}])$$

- Equivalent to reshaping C as 4 index array, then permuting the axis
  $\tilde{C}$= `permute( reshape(C, [mB,mA, nB,nA]), [2, 4, 1,3]);`
- The matrices A, B are obtained from the singular vectors (optimal rank-1 approximation) of matrix $\tilde{C}([ia, ja], [ib, jb]) \approx \sigma_1 \mathbf{a}\mathbf{b}^t$

$$\begin{aligned} C([ib, ia], [\mathbf{jb}, \mathbf{ja}]) &\approx A([ia, \mathbf{ja}]) * B([ib, \mathbf{jb}]) \\ \tilde{C}([ia, \mathbf{ja}], [ib, \mathbf{jb}]) &\approx \sigma_1 \mathbf{a}\mathbf{b}^t \\ &\approx A([ia, \mathbf{ja}]) * B([ib, \mathbf{jb}]) \end{aligned}$$

- C. van Loan, *The Ubiquitous Kronecker Product*, Journal of Computational and Applied Mathematics, 1(**123**), pages 85-100, 2000.

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Generalized Result

- Idea: Rewrite sum of Kronecker products in decreasing importance of Kronecker products.
- Given a sum of Kronecker products, $C = \sum_k^r A_k \otimes B_k$, we can rewrite the same expression as $C = \sum_k^r \sigma_k \tilde{A}_k \otimes \tilde{B}_k$ where $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r \geq 0$ and $\|\tilde{A}_k\|_F = \|\tilde{B}_k\|_F = 1$.
- Result follows from Singular Value Decomposition (SVD) of rearranged matrix E, which has rank r.

$$\begin{aligned}
\tilde{C} &= [A_1(:)|\ldots|A_r(:)]\,[B_1(:)|\ldots|B_r(:)]^t = \mathcal{A}\mathcal{B}^t \\
&= Q_A R_A (Q_B R_B)^t = Q_A (R_A R_B^t) Q_B^t \\
&= Q_A (U D V^t) Q_B^t = (Q_A U) D (Q_B V)^t = \tilde{\mathcal{A}} D \tilde{\mathcal{B}}^t \\
\tilde{C} &= \left[\tilde{A}_1(:)|\ldots|\tilde{A}_r(:)\right] \mathrm{diag}(\sigma_1, \ldots, \sigma_r) \left[\tilde{B}_1(:)|\ldots|\tilde{B}_r(:)\right]
\end{aligned}$$

where QR factorization (or Gram-Schmidt orthogonalization) of $\mathcal{A}$ and $\mathcal{B}$ gives Q_A, Q_B with orthogonal columns with R_A and R_B are $r \times r$ upper triangular matrices

Nearest Kronecker Product

- If A_k or B_k have prescribed sparsity pattern (say A_k is tridiagonal and C is block tridiagonal), we can restrict SVD to non-zero entries
- For example, let A be an $m \times m$ tridiagonal matrix, and $A(:) = Pa$ where $(3m-2) \times 1$ vector a holds the non-zero entries of A, and matrix P $(m^2 \times (3m-2))$ consists of columns of identity matrix that correspond to tridiagonal positions in A. Note that $P^t P$ is the identity matrix of size $(3m-2) \times (3m-2)$.
- Idea: Compute SVD of $P^t \tilde{C}$ $((3m-2) \times nnz(B))$, then expand $\tilde{A}(:) = Pa$
- Adding or removing a Kronecker product is related to up-dating or down-dating the QR factorization of $\mathcal{A}$ and $\mathcal{B}$.

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Preconditioning by Kronecker Products

- If $C \approx A \otimes B$, then $(A \otimes B)^{-1} = (A^{-1} \otimes B^{-1})$ may be an effective preconditioner.
- If $C \approx A_1 \otimes B_1 + A_2 \otimes B_2$, then consider a fast solver for sum of 2 Kronecker products.
- If $C \approx \sum_k^r \tilde{A}_k \otimes \tilde{B}_k$, then rewrite sum in decreasing order of importance and use first few terms as preconditioner.

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Fast Solver for Sum of 2 Kronecker Products

- Fast solver for $C = A_1 \otimes B_1 + A_2 \otimes B_2$ by computing the QZ decomposition of A_1, A_2.
- Find common matrices U_A, V_A to simultaneously transform $U_A * A_1 * V_A = D_{A_1}$, $U_A * A_2 * V_A = D_{A_2}$ to diagonal matrices.
- Solve $Cx = r$ by transforming system to diagonal matrices $U = U_A \otimes U_B$, $V = V_A \otimes V_B$, to solve $UC(Vy) = (Ur)$, $x = Vy$,

$$
\begin{aligned}
UCV &= (U_A \otimes U_B) C (V_A \otimes V_B) \\
&= (U_A \otimes U_B)(A_1 \otimes B_1 + A_2 \otimes B_2)(V_A \otimes V_B) \\
&= (U_A A_1 V_A) \otimes (U_B B_1 V_B) + (U_A A_2 V_A) \otimes (U_B B_2 V_B) \\
&= (D_{A_1} \otimes D_{B_1}) + (D_{A_2} \otimes D_{B_2}), \quad \text{is diagonal.}
\end{aligned}
$$

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QZ Decomposition

- $QZ(A, B)$ generalized eigen decomposition to produce eigenvectors V, triangular $\mathcal{A}$, $\mathcal{B}$, and orthogonal Q, Z, such that $\alpha = \text{diag}(\mathcal{A})$, $\beta = \text{diag}(\mathcal{B})$, $\lambda = \alpha/\beta$,

$$\mathcal{A} = QAZ, \quad \mathcal{B} = QBZ, \quad AV\,\text{diag}(\beta) = BV\,\text{diag}(\alpha)$$

- Let $U = \tilde{U}^{-1}$ where

$$\tilde{U}(:, i) = \begin{cases} AV(:, i) & \text{if } |\alpha_i| \geq |\beta_i| \\ BV(:, i) & \text{otherwise} \end{cases}$$

  then UAV is diagonal, $U(BV\,\text{diag}(\alpha)) = U(AV\,\text{diag}(\beta))$ is also diagonal.
- Problem if V (or $\tilde{U}$) is not full rank or ill-conditioned.

General Sum of Kronecker Products

- No (known) general fast solver for sum of 3 or more Kronecker products.
- Finite difference method for incompressible Navier-Stokes equations on staggered rectangular grid

$$L = C_\ell \otimes C_n \otimes A_m + C_\ell \otimes B_n \otimes C_m + E_\ell \otimes C_n \otimes C_m$$

  where A_m, B_n, E_ℓ, and C matrices are tridiagonal. Derive transformations so that $(I \otimes U_A \otimes U_B)L(I \otimes V_A \otimes V_B)$ is tridiagonal.
- Kamm and Nagy considered the approximation $C = \sum_k^r A_k \otimes B_k \approx UDV'$, for where $U = U_A \otimes U_B$, $V = V_A \otimes V_B$, are obtained from SVD $A_1 = U_A D_A V_A'$, $B_1 = U_B D_B V_B'$ and $D = \mathrm{diag}(U'(C)V)$.
- Ford and Tyrtyshnikov considered a discrete wavelet transform on a sum of Kronecker products ($D = W'CW$, W is wavelet transform) to obtain a sufficiently sparse representation so that a sparse direct solver can be applied.

Resources about Kronecker Products

- *The Ubiquitous Kronecker Product* by C. Van Loan, Journal of Computational and Applied Mathematics, 123(2000), pp. 85-100.
- *Approximation with Kronecker Products* by C. Van Loan and N. Pitsianis in Linear Algebra for Large Scale and Real Time Applications, M. S. Moonen and G. H. Golub, eds., Kluwer Publications, 1993, pp. 293-314. (See also `http://www.cs.duke.edu/~nikos/KP/home.html`).
- *The Kronecker product and stochastic automata networks* by Amy N. Langville and William J. Stewart, J. Comput. Appl. Math., 167(2004) 429-447.
- *Computational Frameworks for the Fast Fourier Transform* by C. Van Loan, SIAM, 1992.

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- *Combining Kronecker product approximation with discrete wavelet transform to solve dense function-related linear systems* by J. M. Ford and E. E. Tyrtyshnikov, SIAM J. Sci. Comput., 25(3):861-981, 2003.
- *A fast Poisson solver for the finite difference solution of the incompressible Navier-Stokes equations* by G. H. Golub, L. C. Huang, H. Simon, W.-P. Tang, SIAM J. Sci. Comput., 19(5):1606-1624,1998.
- *Kronecker product and SVD approximations in image restoration* by J. Kamm and J. G. Nagy, Linear Algebra and its Applications, 284:177-192, 1998.

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Extremescale Computing

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Challenges in Exascale (10^{18})Computing

- The major issue is energy.
- Moving data is the largest cost of energy.
- **It is not about FLOPS. It is about data movement.**
- Exascale machine may have only 64 PBytes of memory
- Need massive amounts ($O(10^9)$ threads) of parallelism. Global synchronization will be very expensive.
- Need to use vectorization (AVX, SSE4 instructions, GPU/MIC accelerator).
- Need attention on fault-tolerance or resilience.

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Algorithm Needs

- Low order FV/FEM, unstructured mesh, incomplete LU preconditioner, classic Krylov with many synchronizations for dot products may not fully exploit future machine
- May need reformulation in
  - regular refinement on grid cells, variables on boundaries of cells
  - high-order discretization
  - parallel in time method
  - relaxed synchronization (asynchronous global sums and dot products)
  - reduce data movement by computing in blocks (e.g. out-of-core algorithm)

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Resources on Exascale Computing

- Workshop reports on exascale applications `http://science.energy.gov/ascr/news-and-resources/program-documents/`
- Scientific Grand Challenges: Fusion Energy Sciences and the Role of Computing at the Extreme Scale, `http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/Fusion_report.pdf`
- International exascale software project, `http://www.exascale.org/iesp/Main_Page`
- Peter M. Kogge (editor), *ExaScale Computing Study: Technology Challenges in Achieving Exascale Systems*, Univ. of Notre Dame, CSE Dept. Tech. Report TR-2008-13, Sept. 28, 2008, `http://www.cse.nd.edu/Reports/2008/TR-2008-13.pdf`
- Extreme-Scale Solvers Workshop, `http://www.orau.gov/extremesolvers2012/`

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Summary

- AORSA wave code uses Fourier basis and requires the parallel solution of large dense complex linear system.
- Current development on 2D anti-aliasing.
- Anderson acceleration (vector extrapolation) for fixed-point iteration using weighted combination of previous iterates.
- Variable separable formulation on rectangular grids commonly leads to Kronecker products.
- Preconditioner based on sum of Kronecker products.
- Extremescale computing will place emphasis on reducing data movement instead of flops.

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