

On Stability of the First Order Newton Schulz Iteration in an Approximate Algebra

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I. INTRODUCTION

In many areas of application, finite correlations lead to matrices with decay properties. By decay, we mean an approximate (perhaps bounded \square) inverse relationship between matrix elements and an associated distance; this may be a simple inverse exponential relationship between elements and the Cartesian distance between support functions, or it may involve a generalized distance, *e.g.* a statistical measure between strings. In electronic structure, correlations manifest in decay properties of the gap shifted matrix sign function, as projector of the effective Hamiltonian (Fig. 1). More broadly, matrix decay properties may correspond to statistical matrices $[? ? ? ? ?]$, including learned correlations in a generalized, non-orthogonal metric \square . More broadly still, problems with local, non-orthogonal support are often solved with congruence transformations of the matrix inverse square root $[? ? ?]$ or a related factorization $[? ?]$; these transformations correlate local support with a representation independent form, *eg.* of the eigenproblem. Interestingly, the matrix sign function and the matrix inverse square root function are related by Higham's identity:

$$\text{sign} \left(\begin{bmatrix} 0 & s \\ I & 0 \end{bmatrix} \right) = \begin{bmatrix} 0 & s^{1/2} \\ s^{-1/2} & 0 \end{bmatrix}. \quad (1)$$

A complete overview of matrix function theory and computation is given in Higham's enjoyable reference $[? ?]$.

A well conditioned matrix s may often correspond to matrix sign and inverse square root functions with rapid exponential decay, and be amenable to the sparse matrix approximation $\bar{s} = s + \epsilon_\tau^s$, where ϵ_τ^s is the error introduced according to some criterion τ . Supporting this approximation are useful bounds to matrix function elements $[? ? ?]$. The criterion τ might be a drop-tolerance, $\epsilon_\tau^s = \{-s_{ij} * \hat{e}_i | |s_{ij}| < \tau\}$, a radial cutoff, $\epsilon_\tau^s = \{-s_{ij} * \hat{e}_i | \|\mathbf{r}_i - \mathbf{r}_j\| > \tau\}$, or some other approach to truncation, perhaps involving a sparsity pattern chosen *a priori*. Then, conventional computational kernels may be employed, such as the sparse general matrix-matrix multiply (SpGEMM) $[? ? ? ?]$, yielding fast solutions for multiplication rich iterations and a modulated (**what do you mean with modulated?**) fill-in. These and

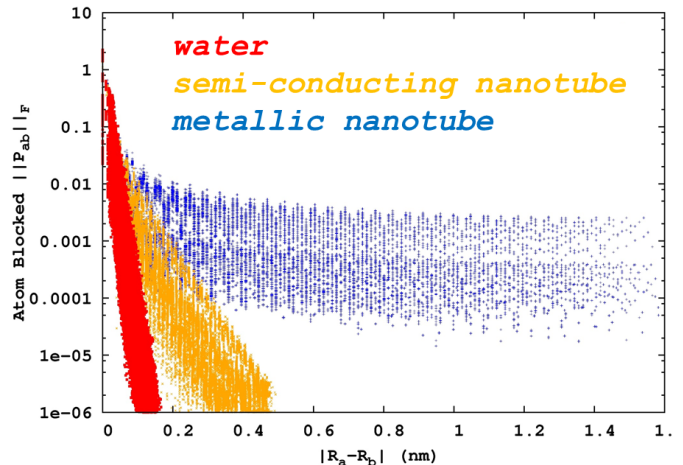


FIG. 1: Examples from electronic structure of decay for the spectral projector (gap shifted sign function) with respect to local (atomic) support. Shown is decay for systems with correlations that are short (insulating water), medium (semi-conducting 4,3 nanotube), and long (metallic 3,3 nanotube) ranged, from exponential (insulating) to algebraic (metallic).

related incomplete/inexact approaches to the computation of sparse approximate matrix functions often lead to $\mathcal{O}(n)$ algorithms, finding wide use in technologically important preconditioning schemes, the information sciences, electronic structure and many other disciplines. Comprehensive surveys of these methods in the numerical linear algebra are given by Benzi $[? ?]$, and by Bowler $[? ?]$ and Benzi $[? ?]$ for electronic structure.

Because the truncated multiplication is controlled only by absolute, additive errors in the product,

$$\overline{a \cdot b} = a \cdot b + \epsilon_\tau^a \cdot b + a \cdot \epsilon_\tau^b + \mathcal{O}(\tau^2) \quad (2)$$

achieving sparse, stable and rapidly convergent iteration for ill-conditioned problems can be challenging \square . In cases of extreme degeneracy, hierarchical semi-seperable (reduced rank) algorithms can offer effective complexity reduction \square . However, many practical cases are somewhere in-between sparse and meaningfully degenerate regimes; effectively dense but without an exploitable reduction in rank. This is the case in electronic structure for strong but non-metallic correlation, *e.g.* towards the Mott transition \square , and also in the case of local atomic support towards completeness $[? ? ? ?]$.

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II. SPARSE APPROXIMATE MATRIX MULTIPLICATION

In this contribution, we consider an N -body approach to the approximation of matrix functions with decay, based on the quadtree data structure [? ?]

$$\mathbf{a}^i = \begin{bmatrix} \mathbf{a}_{00}^{i+1} & \mathbf{a}_{01}^{i+1} \\ \mathbf{a}_{10}^{i+1} & \mathbf{a}_{11}^{i+1} \end{bmatrix}, \quad (3)$$

(I know we argued about this before, but I still like the normal 1-based notation better :)) and orderings that are locality preserving [?]. Orderings that preserve data locality are well developed in the database theory [?], providing fast spatial and metric queries. Locality enabled, fast data access is central to the N -Body

approximation [?], and an important problem for enterprise [?] and runtime systems [?], with memory hierarchies becoming increasingly asynchronous and decentralized [? ?]. For matrices with decay, orderings that preserve locality lead to blocked-by-magnitude matrix structures with well segregated neighborhoods, inhabited by matrix elements of like size, and efficiently resolved by the quadtree data structure [?].

A. Stable SpAMM

With blocked-by-magnitude ordering of matrices \mathbf{a} and \mathbf{b} , the Sparse Approximate Matrix Multiplication (SpAMM) kernel, \otimes_τ , carries out fast occlusion culling of insignificant volumes in the product octree:

$$\mathbf{a}^i \otimes_\tau \mathbf{b}^i = \begin{cases} \emptyset & \text{if } \|\mathbf{a}^i\| \|\mathbf{b}^i\| < \tau \|\mathbf{a}\| \|\mathbf{b}\| \\ \mathbf{a}^i \cdot \mathbf{b}^i & \text{if (i = leaf)} \\ \begin{bmatrix} \mathbf{a}_{00}^{i+1} \otimes_\tau \mathbf{b}_{00}^{i+1} + \mathbf{a}_{01}^{i+1} \otimes_\tau \mathbf{b}_{10}^{i+1}, & \mathbf{a}_{00}^{i+1} \otimes_\tau \mathbf{b}_{01}^{i+1} + \mathbf{a}_{01}^{i+1} \otimes_\tau \mathbf{b}_{11}^{i+1} \\ \mathbf{a}_{10}^{i+1} \otimes_\tau \mathbf{b}_{00}^{i+1} + \mathbf{a}_{11}^{i+1} \otimes_\tau \mathbf{b}_{10}^{i+1}, & \mathbf{a}_{10}^{i+1} \otimes_\tau \mathbf{b}_{01}^{i+1} + \mathbf{a}_{11}^{i+1} \otimes_\tau \mathbf{b}_{11}^{i+1} \end{bmatrix} & \text{else} \end{cases}, \quad (4)$$

with errors linear in τ bounded by the sub-multiplicative norms $\|\cdot\| \equiv \|\cdot\|_F$ and the Cauchy-Schwarz inequality [? ?].

The approximate SpAMM product is

$$\widetilde{\mathbf{a} \cdot \mathbf{b}} \equiv \mathbf{a} \otimes_\tau \mathbf{b} = \mathbf{a} \cdot \mathbf{b} + \Delta_\tau^{a \cdot b} \quad (5)$$

with the culled contractions $\Delta_\tau^{a \cdot b}$ obeying the SpAMM bound

$$\|\Delta_\tau^{a \cdot b}\| \leq \tau \|\mathbf{a}\| \|\mathbf{b}\|, \quad (6)$$

at each level of recursion. This makes \otimes_τ *stable*, as defined by Demmel, Dumitriu and Holz (DDH; Ref. [? ?]). However, instead of the roundoff error, we are concerned with a deterministic SpAMM error¹, which leads to a non-associative algebra and error flows with properties of the Lie bracket

$$[\widetilde{\mathbf{a}}, \widetilde{\mathbf{b}}] \equiv \mathbf{a} \otimes_\tau \mathbf{b} - \mathbf{b} \otimes_\tau \mathbf{a} = [\mathbf{a}, \mathbf{b}] + \Delta_\tau^{a \cdot b} - \Delta_\tau^{b \cdot a}. \quad (7)$$

B. Related Research

Here, we note overlapping themes and research related to the results presented here. First, its worth noting

that the SpAMM concept has evolved, from a row-column based occlusion [?], to recursive octree occlusion [?], and in this work, to the bounded (stable) occlusion satisfying Eq. 6. This evolution cooresponds to an ongoing economization and radical simplification of strongly interacting, high performance solvers in the **freeon** ecosystem [?]. These economizations include n -body algorithms for the five common electronic structure solvers [?], and the (ongoing) development of generic strategies supporting rapid, hierarheical access of spatial and metric data [? ?]. For example, SpAMM has been extended to the *triple* metric query for hextree occlusion of the exact Fock exchange [?].

SpAMM is broadly related to *generalized n-body* methods, popularized by Grey [?], that are simply algorithms based on fast (hierarchical) spatial and metric query [? ?] together with local approximation [?]. Recently, x, y and Yellik showed perfect strong scaling and communication optimality for pairwise n -body methods [? ? ?]. Also Demmel and showed for the related fast matrix multiplication. It may be possible to show similar results, based on the locality of reference developed in this work, encompassing both strong Euclidian locality and with algebraic (diagonal) locality towards identity.

As noted by Aluru [?], the top-down n -body model and breadth-first map-reduction are equivalent [?], offering the potential for alignment with emergent enterprise frameworks [?] and functional programming languages that support generacity [?]. Language support for generic recur-

¹ A non-deterministic SpAMM occlusion error is also possible, *e.g.* associated with probabilistic stabilization [?] or sampling [?] methods.

sion may allow very complex solver ecosystems with very simple (skeletonized) frameworks, lowering barriers to entry, enhancing performance towards decentralized memory landscapes, and following a sustainable commodity trend [?] that offers increasingly cheap compute cycles over the next few decades [?].

SpAMM is perhaps most closely related to the Strassen-like branch of fast matrix multiplication [?], which has been on fire with recent new developments [?]. In the Strassen-like approach, disjoint volumes in (abstract) tensor intermediates are omitted recursively [?]. In the SpAMM approach to fast multiplication, a volume of significant contributions is culled from the naive ijk -cube of the intermediate contraction, with error bounded by Eq. 6. These approaches would seem to be compatible and synergistic.

SpAMM is also related to technologies for the non-deterministic, compressive sampling of the product. These technologies have also seen exciting developments, including sketching [? ?], joining, sensing and probing [?]. These methods involve a wheighted (probablistic) and on the fly sampling with the potential for complexity reduction under certain assumptions (random distributions) [is this true for all? what about MAD?]. SpAMM also employs an on the fly wheighted sampling, based on the product of matrix norms, but operating under the contrary assumption of compression through locality in the naive ijk space, brought about via correlations in the algebra (towards identity) and in the underlying data (blocked-by-magnitude).

Methods that achieve compression in the product stream are different from reduced rank algorithms that achieve matrix compression [?] and/or sparsification [?] of the matrix in a step preceeding multiplication. However, these approaches are not incompatible, with the quadtree data structure supportive of most approaches to matrix compression [?] and sparsification [?], as well as most fast solvers they might interact with. With little deflation in the cost of fast memory, solver ecosystems that can bring multiple levels of approximation to in place data may enjoy significant cumulative advantages.

Finally, the mathematical developments in Higham, Mackey, Mackey and T (HMMT; Ref. [?]) demonstrate the convergence of NS iteration under all groups, addressing potential failure due to the development of pathological symmetries related to *e.g.* Eq. 7. Also in this key paper, HMMT develop the fixed point stability analyses (about 2/3 of the way in), which this work draws heavily upon. This work also draws on the scaling in Chen and Chow's [?] approach to a scaled NS iteration for ill-conditioned problems.

III. FIRST ORDER NEWTON-SHULZ ITERATION

There are two common, first order NS iterations; the sign iteration and the square root iteration, related by

the square, $\mathbf{I}(\cdot) = \text{sign}^2(\cdot)$. These equivalent iterations converge linearly at first, then enter a basin of stability marked by super-linear convergence. Our interest is to access this basin with the most permissive τ possible, building a foundation for future refinement at a reduced cost and with a higher precision ($\tau \rightarrow 0$) [?].

A. Sign iteration

For the NS sign iteration, this basin is marked by a behavioral change in the difference $\delta\mathbf{X}_k = \widetilde{\mathbf{X}}_k - \mathbf{X}_k = \text{sign}(\mathbf{X}_{k-1} + \delta\mathbf{X}_{k-1}) - \text{sign}(\mathbf{X}_{k-1})$, where $\delta\mathbf{X}_{k-1}$ is some previous error. The change in behavior is associated with the onset of idempotence and the bounded eigenvalues of $\text{sign}'(\cdot)$, leading to stable iteration when $\text{sign}'(\mathbf{X}_{k-1})\delta\mathbf{X}_{k-1} < 1$. Global perturbative bounds on this iteration have been derived by Bai and Demmel [?], while Byers, He and Mehrmann [?] developed asymptotic bounds. The automatic stability of sign iteration is a well developed theme in Ref.[?].

B. Square root iteration

In this work, we are concerned with resolution of the identity [?]

$$\mathbf{I}(\mathbf{s}) = \mathbf{s}^{1/2} \cdot \mathbf{s}^{-1/2}, \quad (8)$$

and the cooresponding canonical (dual) square root iteration [?];

$$\begin{aligned} \mathbf{y}_k &\leftarrow h_\alpha[\mathbf{y}_{k-1} \cdot \mathbf{z}_{k-1}] \cdot \mathbf{y}_{k-1} \\ \mathbf{z}_k &\leftarrow \mathbf{z}_{k-1} \cdot h_\alpha[\mathbf{y}_{k-1} \cdot \mathbf{z}_{k-1}] \end{aligned} \quad (9)$$

with eigenvalues in the proper domain aggregated towards 0 or 1 by the NS map $h_\alpha[\mathbf{x}] = \frac{\sqrt{\alpha}}{2}(3 - \alpha\mathbf{x})$ [?]. Then, starting with $\mathbf{z}_0 = \mathbf{I}$ and $\mathbf{x}_0 = \mathbf{y}_0 = \mathbf{s}$, $\mathbf{y}_k \rightarrow \mathbf{s}^{1/2}$, $\mathbf{z}_k \rightarrow \mathbf{s}^{-1/2}$ and $\mathbf{x}_k \rightarrow \mathbf{I}$. As in the case of sign iteration, this dual iteration was shown by Higham, Mackey, Mackey and Tisseur [?] to remain bounded in the superlinear regime, by idempotent Frechet derivatives about the fixed point ($\mathbf{s}^{1/2}, \mathbf{s}^{-1/2}$), in the direction $(\delta\mathbf{y}_{k-1}, \delta\mathbf{z}_{k-1})$:

$$\delta\mathbf{y}_k = \frac{1}{2}\delta\mathbf{y}_{k-1} - \frac{1}{2}\mathbf{s}^{1/2} \cdot \delta\mathbf{z}_{k-1} \cdot \mathbf{s}^{1/2} \quad (10)$$

$$\delta\mathbf{z}_k = \frac{1}{2}\delta\mathbf{z}_{k-1} - \frac{1}{2}\mathbf{s}^{-1/2} \cdot \delta\mathbf{y}_{k-1} \cdot \mathbf{s}^{-1/2} \quad (11)$$

In this contribution, we consider another aspect of convergence, namely the (hopefully) linear approach towards stability of the iteration

$$\widetilde{\mathbf{x}}_k \leftarrow \widetilde{\mathbf{y}}_k(\widetilde{\mathbf{x}}_{k-1}) \otimes_\tau \widetilde{\mathbf{z}}_k(\widetilde{\mathbf{x}}_{k-1}), \quad (12)$$

made difficult by ill-conditioning and a sketchy \otimes_τ .

C. the NS map

Initially, h'_α at the smallest eigenvalue x_0 controls the rate of progress towards idempotence. As recently shown by Jie and Chen [?], for very ill-conditioned problems, a factor of two reduction in the number of NS steps can be achieved by choosing $\alpha \sim 2.85$, which is at the edge of stability. As argued by Pan and Schreiber [?], Jie and Chen [?], switching or damping the scaling factor towards $\alpha = 1$ at convergence is important, shifting emphasis away from the behavior of x_0 towards *e.g.* $x_i \in [0.01, 1]$, emphasizing overall convergence of the broad distribution [?]. In an approximate algebra like SpAMM, the potential for eigenvalues to fluctuate out of the domain of convergence must be considered. This is addressed in Section ??.

D. Instance, Stability and Ill-conditioning

There are a number of nominally equivalent instances of the square root iteration, related by commutations and transpositions. However, these instances may have very different stability properties, controlled to first order by the Frechet derivatives

$$\mathbf{x}_{\delta \hat{\mathbf{y}}_{k-1}} = \lim_{\tau \rightarrow 0} \frac{\mathbf{x}(\mathbf{y}_{k-1} + \tau \delta \hat{\mathbf{y}}_{k-1}, \mathbf{z}_{k-1}) - \mathbf{x}_k}{\tau} \quad (13)$$

and

$$\mathbf{x}_{\delta \hat{\mathbf{z}}_{k-1}} = \lim_{\tau \rightarrow 0} \frac{\mathbf{x}(\mathbf{y}_{k-1}, \mathbf{z}_{k-1} + \tau \delta \hat{\mathbf{z}}_{k-1}) - \mathbf{x}_k}{\tau}, \quad (14)$$

along the unit directions of the previous errors $\delta \hat{\mathbf{y}}_{k-1}$ and $\delta \hat{\mathbf{z}}_{k-1}$, corresponding to the associated displacement magnitudes $\delta y_{k-1} = \|\delta \mathbf{y}_{k-1}\|$ and $\delta z_{k-1} = \|\delta \mathbf{z}_{k-1}\|$. Then, the differential

$$\delta \mathbf{x}_k = \mathbf{x}_{\delta \hat{\mathbf{y}}_{k-1}} \times \delta y_{k-1} + \mathbf{x}_{\delta \hat{\mathbf{z}}_{k-1}} \times \delta z_{k-1} + \mathcal{O}(\tau^2) \quad (15)$$

determines the total first order stability.

This formulation allows to consider orientational effects involving eigenvector fidelity and convergence of derivatives towards zero separately from displacement effects involving accumulation and SpAMM source errors. In some cases, instabilities may be associated with derivatives that do not vanish towards identity, yielding an unbounded iteration []. In other instances, an instability may be associated with rapidly increasing displacements, due to a too large τ . Instability may also arise due to the numerical corruption of the eigenvectors, also resulting in derivatives that vanish too slowly (or blow up altogether).

The potential for instability is increased with ill-conditioning through the terms $\|\mathbf{z}_k\| \rightarrow \sqrt{\kappa(\mathbf{s})}$. Also for ill-conditioned systems, scaling is necessary to accelerate convergence. However with scaling, increasing the map derivative h'_α can also further enhance the rate of error accumulation.

In following sections, we'll examine how these effects differ from the ideal (double precision) canonical (dual) square root iteration for ill-conditioned systems and in the strongly non-associative, sketchy \otimes_τ regime corresponding to permissive values of τ . At this early stage, we are interested in hazards and opportunities associated with different formulations and implementational details. In addition to deviations from the full precision dual instance, we will develop the "stabilized" instance,

$$\begin{aligned} \mathbf{z}_k &\leftarrow \mathbf{z}_{k-1} \cdot h_\alpha[\mathbf{x}_{k-1}] , \\ \mathbf{x}_k &\leftarrow \mathbf{z}_k^\dagger \cdot \mathbf{s} \cdot \mathbf{z}_{k-1} , \end{aligned} \quad (16)$$

with the corresponding differential;

$$\delta \mathbf{x}_k = \mathbf{x}_{\delta \hat{\mathbf{z}}_{k-1}} \times \delta z_{k-1} + \mathcal{O}(\tau^2). \quad (17)$$

Nominally, \mathbf{y}^{dual} is equivalent to $\mathbf{y}_k^{\text{stab}} \equiv \mathbf{z}_k^\dagger \cdot \mathbf{s}$ is also equivalent to $\mathbf{y}_k^{\text{naive}} \equiv \mathbf{z}_k \cdot \mathbf{s}$. However, with ill-conditioning and in only double precision, these two instances may diverge due to rapidly compounding non-associative errors. In the case of the duals iteration under SpAMM approximation, the $\hat{\mathbf{y}}_k^{\text{dual}}$ channel does not retain contact with the eigenvectors, span \mathbf{s} , whilst the stab instance does. In the duals iteration, the $\hat{\mathbf{y}}_k$ SpAMM update is mild, with errors in the relative product remaining well conditioned. In the stab instance, connection with \mathbf{s} is retained at each step, but at the price of the $\mathbf{y}_k^{\text{stab}}$ update involving magnitudes that vary widely in the SpAMM product.

For these reasons, maintaining connection to the eigenvectors of \mathbf{s} through a tighter first product is necessary. In the stab instance, and with a tighter "s" product, $\tau_s \ll \tau$, we find very interesting left/right differences; namely, the right first product

$$\tilde{\mathbf{x}}_k^R \leftarrow \tilde{\mathbf{z}}_k^\dagger \otimes_\tau (\mathbf{s} \otimes_{\tau_s} \tilde{\mathbf{z}}_{k-1}) , \quad (18)$$

is different from the left first product

$$\tilde{\mathbf{x}}_k^L \leftarrow \left(\tilde{\mathbf{z}}_k^\dagger \otimes_{\tau_s} \mathbf{s} \right) \otimes_\tau \tilde{\mathbf{z}}_{k-1} . \quad (19)$$

IV. IMPLEMENTATION

FP, F08, OpenMP 4.0

In the current implementation, all persistence data (norms, flops, branches & *etc.*) are accumulated compactly in the backward recurrence. This persistence data that may be achieved by minimal locally essential trees [].

A. stabilization

B. switching & convergence

Map switching and etc based on TrX

V. DATA

1. double exponential ill-conditioning

3,3 carbon nanotube with diffuse sp -function double exponential (Fig.)

2. three-dimensional, periodic

3. Matrix Market

VI. RESULTS

A. Stability (Proof)

B. Error Flows in Square Root Iteration

1. The canonical (dual) instance

To start, consider just the first order error $\delta \mathbf{x}_k$ that develops from the previous errors $\delta \mathbf{y}_{k-1}$ and $\delta \mathbf{z}_{k-1}$ through the Fréchet derivatives []

$$\mathbf{x}_{\delta \hat{\mathbf{y}}_{k-1}} = \mathbf{y}_{\delta \hat{\mathbf{y}}_{k-1}} \cdot \mathbf{z}_k + \mathbf{y}_k \cdot \mathbf{z}_{\delta \hat{\mathbf{y}}_{k-1}} \quad (20)$$

and

$$\mathbf{x}_{\delta \hat{\mathbf{z}}_{k-1}} = \mathbf{y}_{\delta \hat{\mathbf{z}}_{k-1}} \cdot \mathbf{z}_k + \mathbf{y}_k \cdot \mathbf{z}_{\delta \hat{\mathbf{z}}_{k-1}}. \quad (21)$$

For $\mathbf{x}_{\delta \hat{\mathbf{y}}_{k-1}}$ we have

$$\begin{aligned} \mathbf{y}_{\delta \hat{\mathbf{y}}_{k-1}} &= h_\alpha [\mathbf{x}_{k-1}] \cdot \delta \hat{\mathbf{y}}_{k-1} \\ &\quad + h'_\alpha \cdot \delta \hat{\mathbf{y}}_{k-1} \cdot \mathbf{z}_{k-1} \cdot \mathbf{y}_{k-1} \end{aligned} \quad (22)$$

and

$$\mathbf{z}_{\delta \hat{\mathbf{y}}_{k-1}} = \mathbf{z}_{k-1} \cdot h'_\alpha \delta \hat{\mathbf{y}}_{k-1} \cdot \mathbf{z}_{k-1} \quad (23)$$

yeilding

$$\begin{aligned} \mathbf{x}_{\delta \hat{\mathbf{y}}_{k-1}} &= h_\alpha [\mathbf{x}_{k-1}] \cdot \delta \hat{\mathbf{y}}_{k-1} \cdot \mathbf{z}_k \\ &\quad + h'_\alpha \delta \hat{\mathbf{y}}_{k-1} \cdot \mathbf{z}_{k-1} \cdot \mathbf{y}_{k-1} \cdot \mathbf{z}_k \\ &\quad + \mathbf{y}_k \cdot \mathbf{z}_{k-1} \cdot h'_\alpha \delta \hat{\mathbf{y}}_{k-1} \cdot \mathbf{z}_{k-1}. \end{aligned} \quad (24)$$

Also, for $\mathbf{x}_{\delta \hat{\mathbf{z}}_{k-1}}$ we have

$$\mathbf{y}_{\delta \hat{\mathbf{z}}_{k-1}} = \mathbf{y}_{k-1} \cdot h'_\alpha \delta \hat{\mathbf{z}}_{k-1} \cdot \mathbf{y}_{k-1} \quad (25)$$

and

$$\begin{aligned} \mathbf{z}_{\delta \hat{\mathbf{z}}_{k-1}} &= \delta \hat{\mathbf{z}}_{k-1} \cdot h_\alpha [\mathbf{x}_{k-1}] \\ &\quad + \mathbf{z}_{k-1} \cdot \mathbf{y}_{k-1} \cdot h'_\alpha \delta \hat{\mathbf{z}}_{k-1}, \end{aligned} \quad (26)$$

yeilding

$$\begin{aligned} \mathbf{x}_{\delta \hat{\mathbf{z}}_{k-1}} &= \mathbf{y}_{k-1} \cdot h'_\alpha \delta \hat{\mathbf{z}}_{k-1} \cdot \mathbf{y}_{k-1} \cdot \mathbf{z}_k \\ &\quad + \mathbf{y}_k \cdot \delta \hat{\mathbf{z}}_{k-1} \cdot h_\alpha [\mathbf{x}_{k-1}] \\ &\quad + \mathbf{y}_k \cdot \mathbf{z}_{k-1} \cdot \mathbf{y}_{k-1} \cdot h'_\alpha \delta \hat{\mathbf{z}}_{k-1}. \end{aligned} \quad (27)$$

Closer to a fixed point orbit, $\mathbf{y}_k \cdot \mathbf{z}_{k-1} \rightarrow \mathbf{I}$, $\mathbf{y}_{k-1} \cdot \mathbf{z}_k \rightarrow \mathbf{I}$, $h_\alpha [\mathbf{x}_k] \rightarrow \mathbf{I}$ and $h'_\alpha \rightarrow -\frac{1}{2} [\cdot]$. Then,

$$\mathbf{x}_{\delta \hat{\mathbf{y}}_{k-1}} \rightarrow \delta \hat{\mathbf{y}}_{k-1} \cdot (\mathbf{z}_k - \mathbf{z}_{k-1}) \quad (28)$$

and

$$\mathbf{x}_{\delta \hat{\mathbf{z}}_{k-1}} \rightarrow (\mathbf{y}_k - \mathbf{y}_{k-1}) \cdot \delta \hat{\mathbf{z}}_{k-1}. \quad (29)$$

Equations 28 and 29 illustrate the contractive nature of the NS identity iteration, with directional contributions from $\delta \mathbf{y}_{k-1}$ and $\delta \mathbf{z}_{k-1}$ tightly shut down in the region of superlinear convergence.

In addition to the amplification of previous errors by the Frechet derivatives, errors are compounded to first order in τ by the SpAMM error. Our model develops the τ dependent displacement $\delta \mathbf{z}_{k-1}$ starting with partially unwinding the approximate $\tilde{\mathbf{z}}_{k-1}$;

$$\tilde{\mathbf{z}}_{k-1} = \tilde{\mathbf{z}}_{k-2} \otimes_\tau h_\alpha [\tilde{\mathbf{x}}_{k-2}] \quad (30)$$

$$= \Delta_{\tau}^{\tilde{\mathbf{z}}_{k-2} \cdot h_\alpha [\tilde{\mathbf{x}}_{k-2}]} + \tilde{\mathbf{z}}_{k-2} \cdot h_\alpha [\tilde{\mathbf{x}}_{k-2}] \quad (31)$$

Then,

$$h_\alpha [\tilde{\mathbf{x}}_{k-2}] = h_\alpha [\mathbf{x}_{k-2}] + h'_\alpha \delta \mathbf{x}_{k-2}, \quad (32)$$

leading to

$$\begin{aligned} \delta \mathbf{z}_{k-1} &= \Delta_{\tau}^{\tilde{\mathbf{z}}_{k-2} \cdot h_\alpha [\tilde{\mathbf{x}}_{k-2}]} \\ &\quad + \delta \mathbf{z}_{k-2} \cdot h_\alpha [\tilde{\mathbf{x}}_{k-2}] + h'_\alpha \delta \mathbf{x}_{k-2} \end{aligned} \quad (33)$$

and

$$\tilde{\mathbf{y}}_{k-1} = h_\alpha [\tilde{\mathbf{x}}_{k-2}] \otimes_\tau \tilde{\mathbf{y}}_{k-2} \quad (34)$$

$$= \Delta_{\tau}^{h_\alpha [\tilde{\mathbf{x}}_{k-2}] \cdot \tilde{\mathbf{y}}_{k-2}} + h_\alpha [\tilde{\mathbf{x}}_{k-2}] \cdot \tilde{\mathbf{y}}_{k-2} \quad (35)$$

with

$$\begin{aligned} \delta \mathbf{y}_{k-1} &= \Delta_{\tau}^{h_\alpha [\tilde{\mathbf{x}}_{k-2}] \cdot \mathbf{y}_{k-2}} \\ &\quad + h'_\alpha \delta \mathbf{x}_{k-2} \cdot \mathbf{y}_{k-2} + h_\alpha [\tilde{\mathbf{x}}_{k-2}] \cdot \delta \mathbf{y}_{k-2}, \end{aligned} \quad (36)$$

$$\begin{aligned} \|\delta \mathbf{z}_{k-1}\| &\lesssim \|\mathbf{z}_{k-2}\| \left(\tau \|h_\alpha [\tilde{\mathbf{x}}_{k-2}]\| + h'_\alpha \|\delta \mathbf{y}_{k-2}\| \right) \\ &\quad + \|\delta \mathbf{z}_{k-2}\| \left(\|h_\alpha [\tilde{\mathbf{x}}_{k-2}]\| + \|\mathbf{y}_{k-2}\| \right) \end{aligned} \quad (37)$$

2. The stabilized (stab) instance

in the “stabilized” instance,

$$\hat{\mathbf{y}}_{k-1}^{\text{stab}} = \tilde{\mathbf{z}}_{k-1}^\dagger \otimes_\tau \mathbf{s} \quad (38)$$

$$= \Delta_{\tau}^{\tilde{\mathbf{z}}_{k-1}^\dagger \cdot \mathbf{s}} + (\tilde{\mathbf{z}}_{k-2} \cdot h_\alpha [\tilde{\mathbf{x}}_{k-2}])^\dagger \cdot \mathbf{s} \quad (39)$$

the displacement is

$$\begin{aligned} \delta \mathbf{y}_{k-1}^{\text{stab}} &= \Delta_{\tau}^{\tilde{\mathbf{z}}_{k-1}^\dagger \cdot \mathbf{s}} \\ &\quad + h'_\alpha \delta \mathbf{x}_{k-2}^\dagger \cdot \mathbf{y}_{k-2} + h_\alpha [\tilde{\mathbf{x}}_{k-2}] \cdot \delta \mathbf{y}_{k-2}. \end{aligned} \quad (40)$$

3. Stability Experiments

4. (3,3) nanotubes at $\kappa = 10^{10}$

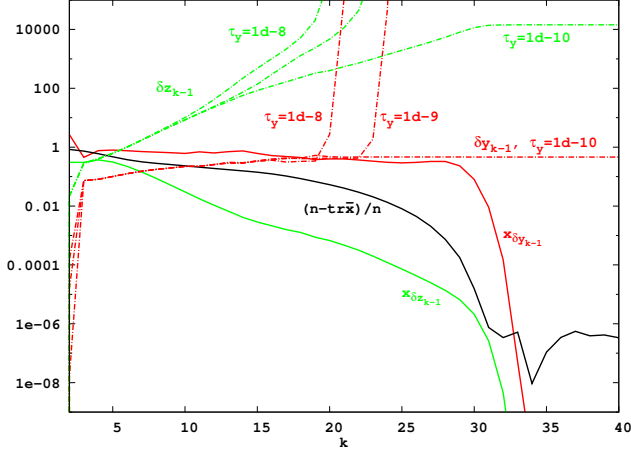


FIG. 2: Derivatives, displacements and the approximate trace of the unscaled, dual NS iteration for a (3,3) nanotube with $\kappa = 10^{10}$. Derivatives are full lines, whilst the displacements cooresponding to $b = 64$, $\tau = 10^{-3}$ and $\tau_y = \{10^{-8}, 10^{-9}, 10^{-10}\}$ are the dashed lines. The trace expectation is shown as a full black line.

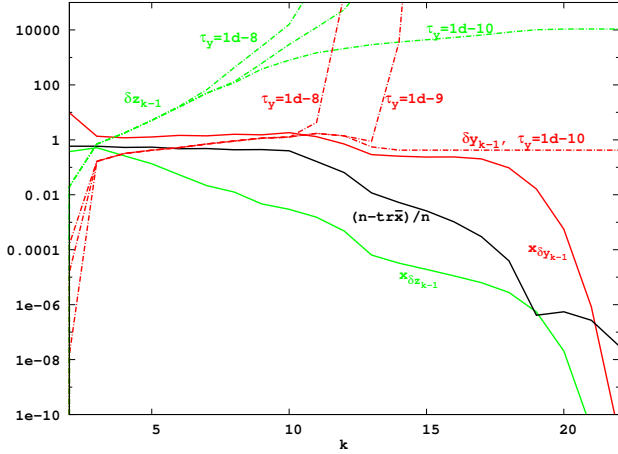


FIG. 3: Derivatives, displacements and the approximate trace of the scaled, stablized NS iteration for a (3,3) nanotube with $\kappa = 10^{10}$. Derivatives are full lines, whilst the displacements cooresponding to $b = 64$, $\tau = 10^{-3}$ and $\tau_y = \{10^{-3}, 10^{-4}, 10^{-6}\}$ are the dashed lines. The trace expectation is shown as a full black line.

5. water boxes

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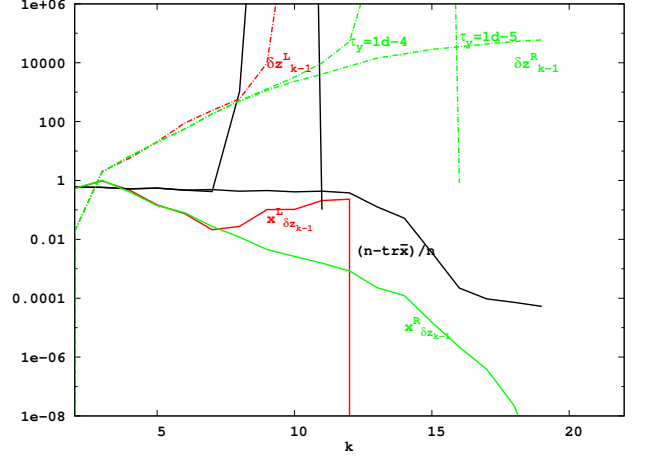


FIG. 4: Derivatives, displacements and the approximate trace of the unscaled, dual NS iteration for a (3,3) nanotube with $\kappa = 10^{10}$. Derivatives are full lines, whilst the displacements cooresponding to $b = 64$, $\tau = 10^{-3}$ and $\tau_y = \{10^{-8}, 10^{-9}, 10^{-10}\}$ are the dashed lines. The trace expectation is shown as a full black line.

FIG. 5: Derivatives, displacements and the approximate trace of the unscaled, stablized NS iteration for a (3,3) nanotube with $\kappa = 10^{10}$. Derivatives are full lines, whilst the displacements cooresponding to $b = 64$, $\tau = 10^{-3}$ and $\tau_y = \{10^{-4}, 10^{-5}, 10^{-6}\}$ are the dashed lines. The trace expectation is shown as a full black line.

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C. Lensing

A feature of square root iteration with the \otimes_τ kernel is localization of the culled octree towards identity iteration, $\tilde{\mathbf{x}}_k \rightarrow \mathbf{I}(\tilde{\mathbf{x}}_{k-1})$. Towards convergence, the product $\tilde{\mathbf{y}}_k \otimes_\tau \tilde{\mathbf{z}}_k$ involves the product of large and small eigenvalues, and large and small norms, which are recursively brought towards unity along the $i = k$ diagonal. Likewise, application of the NS map, Eq. (9), tend towards reflection about the ijk cube-diagonal. Because the SpAMM error obeys the multiplicative Cauchy-Schwarz bound, Eq. (), the cooresponding culled-octree can likewise follow the $i = j$ plane about the ijk cube-diagonal, resolving the *relative* error in identity to within τ . This effect is shown in Figure ???. We call this identity related, plane-wise concentration of the culled octree about the cube-diagonal *lensing*.

Lensing is an algebraic localization offering compression beyond ,

complexity reduction relative to the naive (full) volume of the cube, and also relative to sparsification strategies that preserve only absolute errors, as in Eq. 2. The lensed task space offers an enhanced locality of reference, and may also afford fast methods with costs approaching an

FIG. 6: Derivatives, displacements and the approximate trace of the unscaled, dual NS iteration for a (3,3) nanotube with $\kappa = 10^{10}$. Derivatives are full lines, whilst the displacements coresponding to $b = 64$, $\tau = 10^{-3}$ and $\tau_y = \{10^{-8}, 10^{-9}, 10^{-10}\}$ are the dashed lines. The trace expectation is shown as a full black line.

in-place scalar multiply and copy, *e.g.* as $h_\alpha \rightarrow \mathbf{I}$ in Eq. 9. Our thesis is that many problems in physical and information sciences can be brought to this lensed state, *e.g.* through preconditioning as described here, and maintained as the NS residual is brought to a higher level of precision with a more complete \otimes_τ , and also with respect to an outer simulation loop, *e.g.* coresponding to time iteration.

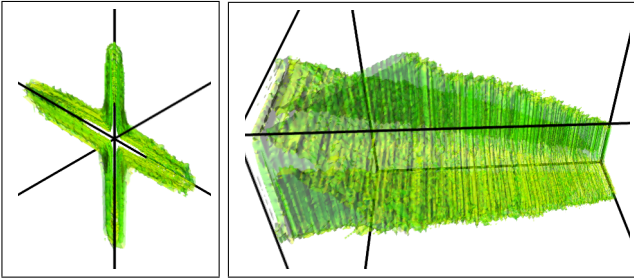


FIG. 7: Views of the $\tau = 0.03$ sign occlusion surface, for the 128x u.c. nanotube, at $\sim 14k \times 14k$ and $\kappa(\mathbf{s}) = 10^6$. This surface envelopes the ijk volume of the \otimes_τ kernel, coresponding to the unscaled dual iteration step $\tilde{\mathbf{x}}_{19} \leftarrow \tilde{\mathbf{y}}_{19 \otimes \tau} \tilde{\mathbf{z}}_{19}$ at $b = 64$, $\tau = 0.03$ and $\tau_y = 10^{-3} \tau$. The first pannel looks straight down the cube-diagonal $i = j = k$, from the upper bound towards (1,1,1). Remarkably, this surface forms an elongated \times , closely following intersection of the $i = j$ and $i = k$ planes along the cube-diagonal. The second pannel looks along the cube-diagonal, with the upper bound at upper left, and (1,1,1) at lower right.

In this section, we present numerical experiments that highlight the effects of ill-conditioning, dimensionality, and the stability of different first order NS approaches to iteration with SpAMM. We turn first to complexity reduction for \otimes_τ in the basin of stability, where we find a novel, compressive effect in the product octree. This

effect is shown in Fig. VIC, for unscaled, inverse square root duals iteration, Eqs. (??), on the 3,3 carbon nanotube metric at $\kappa = 10^6$.

In this example, the SpAMM octree culled from the ijk -cube is outlined by its occlusion surface, enclosing a volume that closely follows the $i = j$ and $i = k$ planes, forming an \times . The banded distribution of large norms along matrix diagonals leads to cube-diagonal dominance, with plane-following a consequence of moderate ill-conditioning, large norms along the plane-diagonals and their overlap in ijk via the multiplicative bound, Eq. (6). The tightness of this bound, and the compression gained relative to methods that control only the absolute error, *e.g.* as given by Eq. (2), will hopefully be quantified in future work.

D. Metric Locality

Metric locality is locality with respect to a Euclidean or generalized distance, *e.g.* of the basis. =====

E. Metric Locality

Metric locality is locality with respect to a Euclidean or generalized distance, *e.g.* of the basis.
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1. unscaled, with hilbert order

2. unscaled, with salesman's order

F. Algebraic Locality

Reflecting about the cube diagonal is copy in place. Cooresponds to lensing.

VII. CONVERSATION