These slides + links to papers: $\underline{\text { hpcgarage.org/futuresparse } 23}$

## Didem, I have bad news for you

## THE FUTURE IS SPARSE

RICH VUDUC - NOVEMBER 17, 2023


https://tenor.com/view/whomp-whomp-whomp-whomp-so-sad-smallest-violin-violin-gif-22252865

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## The future is not sparse



## The future is not sparse



## Four "generations" of computing

| Generation | Time frame | Human-computer ratio | Canonical device | Application |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  | Initial | Follow-on |
| 1 | Mid-1930s | Many-1 | Mainframe | Scientific calculation | Data processing |
| 2 | Late 1960s | 1-1 | PC | Spreadsheet | Database management, document processing |
| 3 | Late 1980s | 1-many | Inch/foot/yard | Calendar and contact management, humanhuman communication | Location-based services, social media, app ecosystem, education |
| 4 | Mid-2000s | Many-many | Cloud/crowd/shroud | Personal navigation and entertainment | Health advisors, educational assistants, supply chain logistics |

## Four "generations" of computing

## OUTLOOK

TABLE 1. A framework for comparing computing generations, inspired by Mark Weiser.

| 4 Generation | Time frame | Human-computer ratio |  | Application |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
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| Rank | System | Cores | (PFlop/s) | (PFlop/s) | (kW) | Top500 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | Frontier - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory <br> United States | 8,699,904 | 1,194.00 | 1,679.82 | 22,703 |  |
| 2 | Aurora - HPE Cray EX - Intel Exascale Compute Blade, Xeon CPU Max 9470 52C 2.4GHz, Intel Data Center GPU Max, Slingshot-11, Intel DOE/SC/Argonne National Laboratory United States | 4,742,808 | 585.34 | 1,059.33 | 24,687 |  |
| 3 | Eagle - Microsoft NDv5, Xeon Platinum 8480C 48C 2GHz, NVIDIA H100, NVIDIA Infiniband NDR, Microsoft Microsoft Azure <br> United States | 1,123,200 | 561.20 | 846.84 |  |  |
| 4 | Supercomputer Fugaku - Supercomputer Fugaku, A64FX 48C <br> 2.2GHz, Tofu interconnect D, Fujitsu <br> RIKEN Center for Computational Science <br> Japan | 7,630,848 | 442.01 | 537.21 | 29,899 |  |
| 5 | LUMI - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC <br> Finland | 2,752,704 | 379.70 | 531.51 | 7,107 |  |


|  | Rank | System | Cores | Rmax (PFlop/s) | Rpeak (PFlop/s) | Power (kW) | Top500 Nov. '23 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
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| 3 | Eagle - Mi <br> NVIDIA H1 <br> Microsoft <br> United Sta | rosoft NDv5, Xeon Platinum 8480C 48C 2GHz O, NVIDIA Infiniband NDR, Microsoft zure es |  | 1,123,2 | 0 | 561.20 | 846.84 |

## Myth 12: All HPC Will Be Subsumed by the Clouds!

The rapidly advancing AI and new precision options has reignited the cloud discussion. The question whether clouds will subsume supercomputing has been ongoing for more than a decade, since the late 2000s Deelman et al. (2008), but remains inconclusive. Today's cloud offerings offer a wide spectrum for HPC customers, ranging from low-cost standard virtual machines to snecialized ton-oear HPC enuinment in

## Al is emerging as "big science" in the tradition of nuclear and high energy physics

| Model size (params) | Training tokens (round) | Training data used (estimate) |
| :---: | :---: | :---: |
| Chinchilla/ |  |  |
| 70B | 1.4 Trillion | 2.3 TB |
| 250B | 5 Trillion | 8.3TB |
| 5008 | 10 Trillon | 16.6 TB |
| $1 T$ | 20 Trillion | 33.3 TB |
| 10 T | 200 Trillion | зз3тв |
| 100T | 2 Quadrillion | 3.3PB |
| 2501 | 5 Quadrillion | 8.3PB |
| 5007 | 10 Quadrillion | 16.6PB |



The scale of needed human and computational resources is beginning to reshape leadership in science

From: SC23 talk by Rick Stevens (Argonne National Lab)


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Q: Can these models be sparse?

A: Yes, but ML sparse is "fake" sparse.


Fig. 4. Typical test error vs. sparsity showing Occam's hill (network: ResNet-50 on Top-1 ImageNet).

Hoefler et al. (2021). "Sparsity in Deep Learning: ... arXiv:2102.00554
Frantar et al. (2023). "Scaling laws for sparsely-connected foundation models. arXiv:2309.08520v1


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Sparse mat-vec (SELL-C- $\sigma$ ) performance rises quickly with density


Sparse mat-vec (SELL-C- $\sigma$ ) performance rises quickly with density


Conclusion so far:
Q: What system will be built for HPC?
A: One for dense (and fake sparse) foundation models.

Q: What is an optimal machine for that case?


Mike Isaev (GT Ph.D.), Nic McDonald (NVIDIA), r. Vuduc (SC23)




Mike Isaev (GT Ph.D.), Nic McDonald (NVIDIA), R. Vuduc (SC23)

## Canonical structure of a large language model



Figure 1: The transformer block structure of Megatron

## Myriad ways to map an LLM to a machine...


(a) Data Parallelism

(b) Model Parallelism

(c) Layer Pipelining

Fig. 14. Neural Network Parallelism Schemes

| Optimization | Year | Related <br> system | Comp <br> time | Comp <br> util | Mem <br> time | Mem <br> cap | Mem <br> BW | Net <br> time | Net <br> BW | range |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Data parallelism (DP) [61] | 1989 | network | - | $\uparrow$ | - | $\uparrow \uparrow \uparrow$ | - | $\uparrow$ | $\uparrow$ | $1 .$. batch |
| DP overlap [25] | 2017 | network | $\uparrow$ | $\downarrow$ | - | - | - | $\downarrow \downarrow \downarrow$ | - | true/false |
| Optimizer sharding [24] | 2019 | network | $\downarrow$ | - | - | $\downarrow \downarrow$ | - | - | - | true/false |
| Recompute [5, 10] | 2000 | compute | $\uparrow \uparrow$ | - | - | $\downarrow \downarrow \downarrow$ | - | - | - | full/attn/none |
| Fused layers [28] | 2018 | compute | - | $\uparrow \uparrow$ | $\downarrow \downarrow$ | $\downarrow \downarrow$ | $\downarrow$ | - | - | true/false |
| Microbatch training [13] | 2019 | compute | - | $\uparrow \uparrow$ | - | $\uparrow \uparrow \uparrow$ | - | - | - | 1 .. batch/DP |
| Pipeline parallelism (PP) [7, 13] | 2012 | network | $\uparrow$ | $\downarrow \downarrow$ | - | $\downarrow \downarrow$ | - | $\uparrow$ | $\uparrow$ | $1 .$. blocks |
| PP 1F1B schedule [7, 32] | 2012 | network | - | - | - | $\downarrow \downarrow$ | - | - | - | true/false |
| PP interleaving [33] | 2021 | network | $\downarrow$ | $\uparrow \uparrow$ | - | $\uparrow$ | - | $\uparrow$ | $\uparrow \uparrow$ | 1 .. blocks/PP |
| PP RS + AG [21] | 2022 | network | - | - | - | - | - | $\downarrow$ | $\downarrow \downarrow$ | true/false |
| Tensor parallelism (TP) [7, 22, 49] | 2012 | network | $\downarrow \downarrow$ | $\downarrow$ | - | $\downarrow \downarrow$ | $\downarrow \downarrow$ | $\uparrow \uparrow \uparrow$ | $\uparrow \uparrow \uparrow$ | $1 .$. attn |
| TP RS + AG instead AR [33] | 2021 | network | - | - | $\uparrow$ | $\uparrow$ | - | $\downarrow$ | $\downarrow$ | true/false |
| Sequence parallelism (SP) [21] | 2022 | network | $\downarrow$ | - | $\downarrow$ | $\downarrow \downarrow$ | $\downarrow$ | $\uparrow$ | $\uparrow$ | true/false |
| TP redo for SP [21] | 2022 | network | - | - | - | $\downarrow$ | - | $\uparrow$ | $\uparrow$ | true/false |
| TP overlap [58] | 2022 | network | $\uparrow$ | $\downarrow$ | - | - | - | $\downarrow \downarrow$ | - | true/false |
| Weight offload [48] | 2021 | memory | - | - | $\uparrow$ | $\downarrow \downarrow \downarrow$ | $\uparrow$ | - | - | true/false |
| Activation offload [48] | 2021 | memory | - | - | $\uparrow$ | $\downarrow \downarrow \downarrow$ | $\uparrow$ | - | - | true/false |
| Optimizer offload [48] | 2021 | memory | - | - | $\uparrow$ | $\downarrow$ | $\uparrow$ | - | - | true/false |

Calculon results compared to State-of-the-Art



| FW pass | FW recompute |
| :--- | :--- | :--- |
| BW pass | TP comm |
| Optim step | PP comm |
| PP bubble | DP comm |



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Calculon results compared to State-of-the-Art


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Calculon results compared to State-of-the-Art


Mike Isaev (GT Ph.D.), Nic McDonald (NVIDIA), R. Vuduc (Sc23)

Q: What is an optimal machine for foundation models?

A: One tuned for dense compute ("big" procs) and slow communication, i.e., a litte HBM, a lot of slow capacity mem, fast on-node network, slow internode network.


Q: What is an optimal machine for foundation models?

A: One tuned for dense compute ("big" procs) and slow communication, i.e., a litte HBM, a lot of slow capacity mem, fast on-node network, slow internode network.


## So, now what?

DESPITE EVERYTHING I JUST SAID THE FUTURE *SHOULD* BE SPARSE!


Recall:

$$
\mathcal{O}\left(N^{2}\right) \longrightarrow \mathcal{O}(N)
$$

Reduces energy: fewer flops, less storage

Recall:

$$
\mathcal{O}\left(N^{2}\right) \longrightarrow \mathcal{O}(N)
$$

## \% time communicating increases

Algorithms for 2D Poisson Equation with N unknowns

| Algorithm | Serial | PRAM | Memory | \#Procs | (Keyes '04) |
| :---: | :---: | :---: | :---: | :---: | :---: |
| - Dense LU | $\mathrm{N}^{3}$ | N | $\mathrm{N}^{2}$ | $\mathbf{N}^{2}$ |  |
| - Band LU | $\mathrm{N}^{2}$ | N | $\mathrm{N}^{3 / 2}$ | N | 1947 |
| - Jacobi | $\mathrm{N}^{2}$ | N | N | N | 1950 |
| - Explicit Inv. | $\mathrm{N}^{2}$ | $\boldsymbol{\operatorname { l o g }} \mathbf{N}$ | $\mathrm{N}^{2}$ | $\mathrm{N}^{2}$ |  |
| - Conj.Grad. | $\mathrm{N}^{3 / 2}$ | $N^{1 / 2} \log N$ | N | N | 1971 |
| - RB SOR | $\mathrm{N}^{3 / 2}$ | N ${ }^{1 / 2}$ | N | N |  |
| - Sparse LU | $\mathrm{N}^{3 / 2}$ | N ${ }^{1 / 2}$ | $N^{*} \log \mathrm{~N}$ | N | ~ 1970s |
| - FFT | $N^{*} \log N$ | $\boldsymbol{\operatorname { l o g }} \mathrm{N}$ | N | N |  |
| - Multigrid | N | $\log ^{2} \mathbf{N}$ | N | N | 1984 |
| - Lower bound | N | $\log N$ | N |  |  |

PRAM is an idealized parallel model with zero cost communication


PRAM is an idealized parallel model with zero cost communication

# Suggestion: Consider sparse LU (+ APSP) as a hardware design target (dense-ish \& sparse-ish) 

## An algorithm

## A communication-avoiding sparse direct solver

Thesis: Significant, and even asymptotic, improvements in the strong scaling of
sparse direct solvers for linear systems and all-pairs shortest paths are possible
by trading more storage for less communication.


Piyush Sao
@piyush314 / ORNL


Xiaoye (Sherry) Li
LBNL


Ramki Kannan
ORNL

$A x=b$


$$
\operatorname{nnz}(A)=\mathcal{O}(N)
$$



## $P A=L U$


$L=$ unit lower triangular
$U=$ upper triangular
$P=$ permutation (pivoting)


$$
\begin{aligned}
L y & =P b & & \text { (forward) } \\
U x & =y & & \text { (backward) }
\end{aligned}
$$



## Aside: All-pairs shortest paths ~ LU but in the tropical semiring

```
FLoydWarshall( \(W\) )
\(1 \quad\) for \(1 \leq i, j \leq n\)
\(2 \quad c_{i, j} \leftarrow w_{i, j}\)
3 for \(1 \leq r \leq n\)
    for \(1 \leq i, j \leq n\)
\(5 \quad c_{i, j} \leftarrow c_{i, j} \oplus\left[c_{i, r} \odot c_{r, j}\right]\)
6 return \(C \equiv\left[c_{i, j}\right]\)
```



Same machinery applies! Reorderings, supernodes, elimination trees, data structures, distribution, GPUs, ... Gordon Bell Finalist (SC20 \& SC22)

## Sparse LU has rich computational structure



## Parallel dependencies = "elimination tree"



Same machinery applies! Reorderings, supernodes, elimination trees, data structures, distribution, GPUs, ... Gordon Bell Finalist (SC20 \& SC22)

## E-tree is really a (fine-grained) task DAG



## E-tree is really a (fine-grained) task DAG



## Tasks have a complex mix of intensities (flop:byte)

1 flop:8 bytes


## "2D" algorithm (strong scaling)

$\begin{array}{cccccccc}-1 & 0.036 & 0.044 & 0.055 & 0.065 & 0.064 & 0.073 & \begin{array}{l}\text { Teraflop/S } \\ (32 x \text { procs } \rightarrow 2 x \text { speedup) }\end{array} \\ 24 & 48 & 96 & 192 & 384 & 768 & \end{array}$
MPI processes (2D process grid; 4 cores / process)

## \# MPI procs



## Example:

$$
P_{x} \times P_{y}=96
$$

(Best configuration shown)

## Teraflop/s

(32x procs $\rightarrow 2 x$ speedup)

MPI processes (2D process grid; 4 cores / process)

## SaO: CA For Sorrse tu (2019-2022)

(communication avoidance)
All known "3D-LU" algorithms ${ }^{\dagger}$ are for dense LU. They reduce communication volume but increase latency.

For sparse LU, we can reduce both the latency and bandwidth for "planar" problems asymptotically, and achieve constant-factor reductions for "non-planar" ones.

There are other memory-for-communication techniques, $\ddagger$ including multifrontal methods. We claim better memory and process scalability. See our papers!
$\dagger$ Ashcraft (1991); Irony \& Toledo (2002); Solomonik \& Demmel (2011)
$\ddagger$ Hulbert \& Zmijewski (1991); Gupta et al. (1997)


(For experts) How? Partition elimination tree among 2-D slides of a 3-D process grid

## Piyush: Extend to sparse LU

## Example:

$$
P_{x} \times P_{y}=96
$$

(Best configuration shown)

## Teraflop/s

(32x procs $\rightarrow 2 x$ speedup)

MPI processes (2D process grid; 4 cores / process)




MPI processes (2D process grid; 4 cores / process)


MPI processes (2D process grid; 4 cores / process)

## Summary

Assume that industry will not build you an efficient machine for your truly sparse computations.

Maybe we should band together around a common set of such computations that can drive hardware design projects. I have suggested sparse LU (sparse APSP) as one whose characteristics-semi-irregular parallelism, dynamic structure, variable intensity-makes it one "model problem" for co-design, but there can, and should, be many others, including yours!


## Bonus / Outtakes / BTS

# Why deep learning may be intrinsically "dense" 

Multiple regression

$$
X \equiv\left[\begin{array}{ccccc}
\mid & \mid & \mid & & \mid \\
x_{i, 0} & x_{i, 1} & x_{i, 2} & \ldots & x_{i, n-1} \\
\mid & \mid & \mid & & \mid
\end{array}\right]
$$

~ Accuracy

~ Ops (~ time)


Linear regression example: Thompson et al., "The computational limits of deep learning" (July 2020). arXiv:2007.05558v1

More samples $\rightarrow$ More accuracy, reasonable time



Linear regression example: Thompson et al., "The computational limits of deep learning" (July 2020). arXiv:2007.05558v1

## Accuracy plateaus and costs rise



Linear regression example: Thompson et al., "The computational limits of deep learning" (July 2020). arXiv:2007.05558v1

With enough data, more accuracy but a high cost
~ Accuracy
2.5. Oracle
~ Ops (~ time)


Linear regression example: Thompson et al., "The computational limits of deep learning" (July 2020). arXiv:2007.05558v1

## Better accuracy with fewer samples, but still expensive



Linear regression example: Thompson et al., "The computational limits of deep learning" (July 2020). arXiv:2007.05558v1


Chunxing Yin (GT Ph.D.), D. Zheng (Amazon), I. Nisrat, C. Faloutsos, G. Karypis, R. Vuduc.
"Nimble GNN embedding with tensor-train decomposition." In KDD'22. doi:10.1145/3534678.3539423


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## Communication avoidance 101

## Communication-avoiding idea

For matrix multiplication, $\boldsymbol{C}+=\boldsymbol{A} \cdot \boldsymbol{B}$, on $\boldsymbol{P}$ processors


# Communication-avoiding idea 

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# Communication-avoiding idea 

For matrix multiplication, $\boldsymbol{C}+=\boldsymbol{A} \cdot \boldsymbol{B}$, on $\boldsymbol{P}$ processors

|  | $B$ |  |
| :---: | :---: | :---: |
|  |  | $N \times N$ matrices $P$ processes |
|  |  | Time for flops $\propto \frac{N^{3}}{P}$ |
| A | C |  |

## Communication-avoiding idea

For matrix multiplication, $\boldsymbol{C}+=\boldsymbol{A} \cdot \boldsymbol{B}$, on $\boldsymbol{P}$ processors


2D process grid

# Communication-avoiding idea 

For matrix multiplication, $\boldsymbol{C}+=\boldsymbol{A} \cdot \boldsymbol{B}$, on $\boldsymbol{P}$ processors


## Communication-avoiding idea

For matrix multiplication, $\boldsymbol{C}+=\boldsymbol{A} \cdot \boldsymbol{B}$, on $\boldsymbol{P}$ processors


Attained by Cannon's algorithm (1969), for instance

## Communication-avoiding idea

For matrix multiplication, $\boldsymbol{C}+=\boldsymbol{A} \cdot \boldsymbol{B}$, on $\boldsymbol{P}$ processors


## Communication-avoiding idea

For matrix multiplication, $\boldsymbol{C}+=\boldsymbol{A} \cdot \boldsymbol{B}$, on $\boldsymbol{P}$ processors


## 3D process grid <br> $$
P=P_{x} \cdot P_{y} \cdot P_{z}
$$

## Communication-avoiding idea

For matrix multiplication, $\boldsymbol{C}+=\boldsymbol{A} \cdot \boldsymbol{B}$, on $\boldsymbol{P}$ processors


Idea: Use a 3-D process grid and replicate Dekel et al. (1981); Agarwal et al. (1995); + more

## Communication-avoiding idea

For matrix multiplication, $\boldsymbol{C}+=\boldsymbol{A} \cdot \boldsymbol{B}$, on $\boldsymbol{P}$ processors


Trades more memory for less communication

## Piyush: CA for sparse LU

All known "3D-LU" algorithms ${ }^{\dagger}$ are for dense LU. They reduce communication volume but increase latency.

For sparse LU, we can reduce both the latency and bandwidth for "planar" problems asymptotically, and achieve constant-factor reductions for "non-planar" ones.

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An "iron law"

## An Iron Law of Parallel and Distributed Computation

A modern cluster or supercomputer is, to first order, a collection of processing nodes. Each node has a processor ("xPU") and a two-level memory hierarchy. Nodes are connected by a network.

As a program executes on this system, it incurs two types of communication cost.
"Vertical" communication occurs in the memory system between, say, RAM and cache.
"Horizontal" communication occurs between nodes across the network.


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"Horizontal" communication occurs between nodes across the network.

(Asymptotic running time - rules-of-thumb)
(Asymptotic running time - rules-of-thumb)

## Compute time

$W(n)$
$P$
(Asymptotic running time - rules-of-thumb)

## Compute time

## $W(n)$

$P$

## P-fold <br> speedup, ideally

(Asymptotic running time - rules-of-thumb)

## Compute time

## $W(n)$ <br> $P$

## Memory

 time

P-fold speedup, ideally
(Asymptotic running time - rules-of-thumb)

## Compute time

## $\underline{W(n)}$ <br> $P$

Memory time

P-fold speedup, ideally

(Asymptotic running time - rules-of-thumb)

## Compute time

## Memory time

## Network time

## $W(n)$ <br> $P$


P-fold speedup, ideally

e.g.,

(Asymptotic running time - rules-of-thumb)

## Compute time

## $W(n)$ <br> $P$

P-fold speedup, ideally

Memory time

## Network time


e.g.,




Asymptotic reduction
(Asymptotic running time - rules-of-thumb)

## Compute time <br> Memory time



## Network time



## DPUs in modern clusters

The basic building block of a distributedmemory cluster or supercomputer is a node.

Each node includes a host, which is a processor (xPU) + memory hierarchy.

The host can communicate with other hosts via its NIC (network interface controller).

A network connects the nodes. The nodes may be arranged in some topology, which determines the network's carrying capacity and cost.

In a smartNIC, the NIC becomes "host-like" via the addition of processing (ypu) and memory.

Node


## Hypothetical: Multi-SmartNIC

## One host xPU (16 cores)

| Mem |
| :---: |
| $\$$ |
|  |
| xPU |

## Hypothetical: Multi-SmartNIC

One host xPU (16 cores)


## 657 GF/s

## Hypothetical: Multi-SmartNIC

One host xPU (16 cores)


## 657 GF/s <br> 76.8 GB/s

## Hypothetical: Multi-SmartNIC



$$
657 \text { GF/s }
$$

$$
76.8 \text { GB/s }
$$

## Hypothetical: Multi-SmartNIC



$$
\begin{aligned}
& 657 \mathrm{GF} / \mathrm{s} \\
& 76.8 \mathrm{~GB} / \mathrm{s}
\end{aligned}
$$

## Hypothetical: Multi-SmartNIC



## Hypothetical: Multi-SmartNIC

One host xPU (16 cores)

~ 8.5 F:B
$8 \times$ BF-2 yPUs (no host)


## Hypothetical: Multi-SmartNIC

One host xPU (16 cores)


Time = "1"
using all cores
$8 \times$ BF-2 yPUs (no host)


## Speedup ~ 1.7x

Real measurement on MiniMD!

## What else could one build?

## Power allocation for an "optimal" matrix multiply machine



## Power allocation for an "optimal" matrix multiply machine



ORNL Summit (13-14 MW):
67.0\% GPU compute 14.9\% CPU compute
4.8\% memory
5.3\% network + disk

8\% node overhead

System Power (MW)

## Power allocation for an "optimal" 3D FFT machine?

## Power allocation for an "optimal" 3D FFT machine



## 3D FFT vs. "Stencil" machines




Relative time (slowdown)


Relative time (slowdown)


Relative time (slowdown)

of the applications. AGILE system designs must emphasize optimization of the fully integrated system rather than independent optimization of individual functionalities (e.g., memory, computation, or communication), and must not be constrained by existing component interfaces and protocols, legacy architectures, or current practices.
A fundamental rethinking of computer architectures that can revitalize performance growth trends in computing capabilities is long overdue. Currently, there is a renewed interest in developing specialized hardware components. However, this approach will not resolve the fundamental data movement challenges that restrict the historical performance growth trends. The AGILE program will seed a new generation

The AGILE BAA was released in November 2021 and the program is slated to run for three years.

## TESTING AND EVALUATION PARTNERS

- Lawrence Berkeley National Laboratory
- Sandia National Laboratory
- Pacific Northwest National Laboratory


## KEYWORDS

- Computer Architecture
- Data analytics
- Co-Design
- Data movement
- Modeling and simulation

