# Algorithm Design at Scale: Porting Parallel FFT-based Fortran Simulations to GPUs

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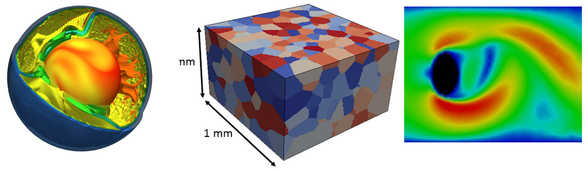
## GPUs for Scientific Computing

General Purpose GPU for scientific computing:
- provide a lot of compute power
- are relatively cheap compared to large clusters.




However, accelerating legacy Fortran scientific codes with GPUs involves **rewriting and rethinking**.
For eg., consider the large memory requirements of the simulation (see table) and memory constraints of GPUs (few GB on-chip).

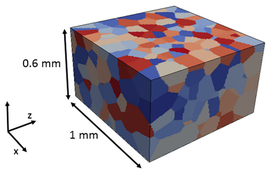
**Hooke's Law Simulation**

| Input data size | $32^3$ | $64^3$ | $128^3$ | $256^3$ | $512^3$ | $1024^3$ |
|---|---|---|---|---|---|---|
| Memory required (GB) | 0.07 | 0.55 | 4.44 | 35.5 | 284 | 2272 |

## Hooke's Law Simulation: Scaling Parallel FFTs

**3D Hooke's law simulates stress and strain (3x3 tensors) in crystals:**

$$\underset{\text{stress}}{\sigma_{ij}} = \underset{\text{3x3x3x3 stiffness tensor}}{C_{ijkl}} : \underset{\text{strain}}{\epsilon_{kl}}$$




**Partial Differential Equation:**

$$C^0_{ijkl} u_{k,lj}(\mathbf{x}) + \tau_{ij,j}(\mathbf{x}) = 0$$

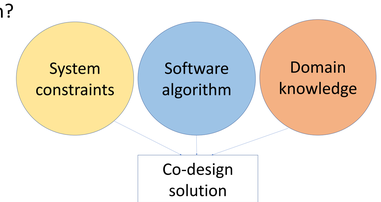
**Original method by Moulinec and Suquet**

1: **Initialize:**
  $\epsilon^0 \leftarrow E$,
  $\sigma^0_{mn}(\mathbf{x}) \leftarrow C_{mnkl}(\mathbf{x}) : \epsilon^0_{kl}(\mathbf{x})$
2: **while** $e_s > e_{tol}$ **do**
3: $\hat{\sigma}^i_{mn}(\boldsymbol{\xi}) \leftarrow \text{FFT}(\sigma^i_{mn}(\mathbf{x}))$
4: Check convergence
5: $\Delta\hat{\epsilon}^{i+1}_{kl}(\boldsymbol{\xi}) \leftarrow \hat{\Gamma}_{klmn}(\boldsymbol{\xi}) : \hat{\sigma}^i_{mn}(\boldsymbol{\xi})$
6: Update strain: $\hat{\epsilon}^{i+1}_{kl}(\boldsymbol{\xi}) \leftarrow \hat{\epsilon}^i_{kl}(\boldsymbol{\xi}) - \Delta\hat{\epsilon}^{i+1}_{kl}(\boldsymbol{\xi})$
7: $\epsilon^{i+1}_{kl}(\mathbf{x}) \leftarrow \text{IFFT}(\hat{\epsilon}^{i+1}_{kl}(\boldsymbol{\xi}))$
8: Update stress: $\sigma^{i+1}_{mn}(\mathbf{x}) \leftarrow C_{mnkl}(\mathbf{x}) : \epsilon^{i+1}_{kl}(\mathbf{x})$

Increasing grid resolution leads to larger problem sizes.

Large parallel FFTs = **prohibitive memory requirement and all-all communication**.

Current MPI simulation limit is $1024^3$ grid
Can using GPUs help us scale this further with a co-design solution?




Images:
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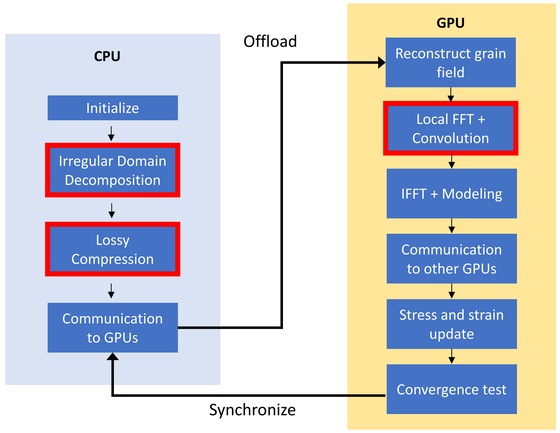
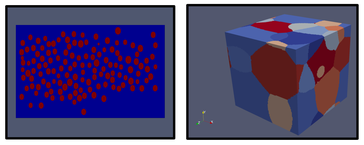
https://www.researchgate.net/profile/Tamas_Csanadi/publication/311421026/figure/fig2/AS:489562741972997@1493732261970/ Effect-of-load-and-crystal-orientation-on-crack-formation-during-scratch-test-b.ppm
https://nvidia.com

## Co-design Solution

**This work presents algorithm development and analysis of the proposed solution in MATLAB.**




**Irregular domains:** Microstructure is decomposed into grains, which are the irregular domains. We are working with 2D and 3D spherical domains, elliptical domains, triangular/polygonal domains and cubic domains.

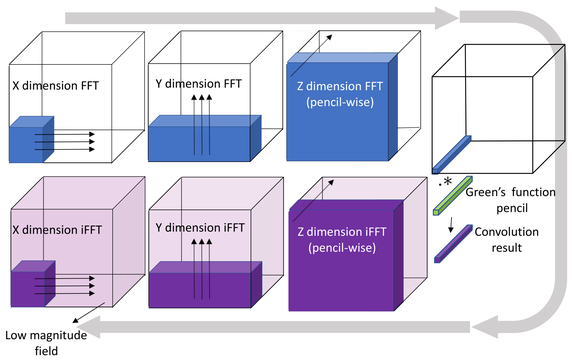


**Lossy compression:** Adaptive downsampling used to reduce storage of convolution result. Sampling strategy is chosen based on desired reconstruction accuracy and a given prior on the field being sampled. For example, from the Eshelby solution, we could have:

**Eshelby tensors**

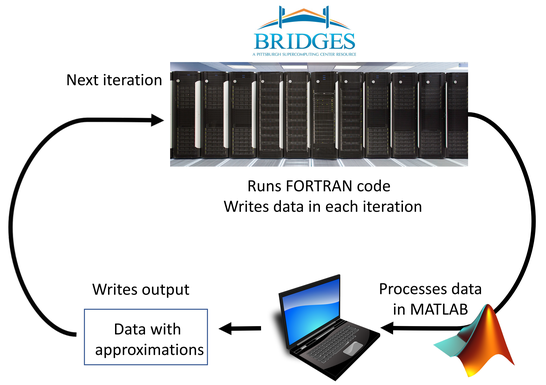
$$\begin{aligned}8\pi(1-\nu)D_{ijkl}(x) =& 8\pi(1-\nu)S_{ijkl}(\lambda) + 2\nu\delta_{kl}x_i I_{I,j}(\lambda) \\ &+(1-\nu)\left(\delta_{il}x_k I_{K,j}(\lambda) + \delta_{jl}x_k I_{K,i}(\lambda)\right. \\ &\left.+\ \delta_{ik}x_l I_{L,j}(\lambda) + \delta_{jk}x_l I_{L,i}(\lambda)\right) \\ &-\delta_{ij}x_k\left(I_K(\lambda) - a_I^2 I_{KI}(\lambda)\right)_{,l} \\ &-(\delta_{ik}x_j + \delta_{jk}x_i)\left(I_J(\lambda) - a_I^2 I_{IJ}(\lambda)\right)_{,l} \\ &-(\delta_{il}x_j + \delta_{jl}x_i)\left(I_J(\lambda) - a_I^2 I_{IJ}(\lambda)\right)_{,k} \\ &-x_i x_j\left(I_J(\lambda) - a_I^2 I_{IJ}(\lambda)\right)_{,lk}.\end{aligned}$$

**Domain-local FFT** on GPU for each domain. Platform used is MATLAB-GPU interface, using **NVIDIA Quadro K2200.**

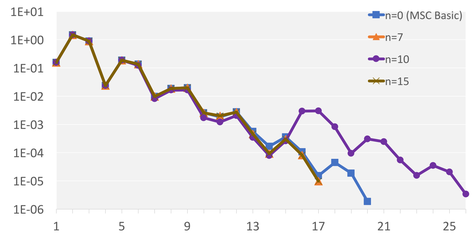



## Phase I: Successes

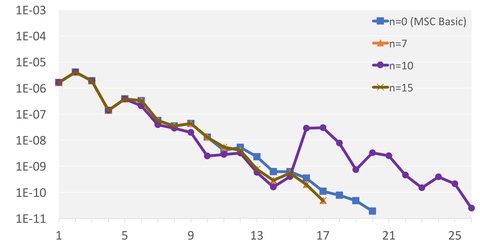
**Computational aspects for prototype development**: **MATLAB-FORTRAN workflow** for convergence analysis is as follows.




**Convergence of Stress**
Log Error in Stress field vs. Iteration number



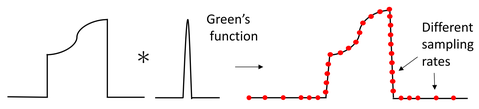

**Convergence of Strain**
Log Error in Strain field vs. Iteration number



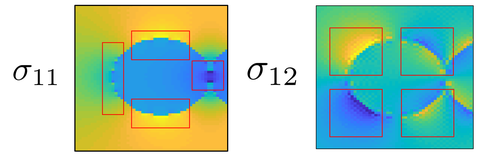

**MATLAB-GPU** Interface to obtain proof-of-concept results for domain-local FFTs. 700 x 700 x 700 size convolution possible grain-by-grain with irregular domain decomposition on NVIDIA Quadro K2200 with 640 CUDA cores and 4 GB GPU memory.

| Grain size | $64^3$ | $128^3$ | $128^2 \times 8$ | $256^2 \times 8$ | $512^2 \times 8$ |
|---|---|---|---|---|---|
| Error(%) | 1.79 | 3.03 | $3.74 \cdot 10^{-14}$ | $4.11 \cdot 10^{-14}$ | $4.32 \cdot 10^{-14}$ |

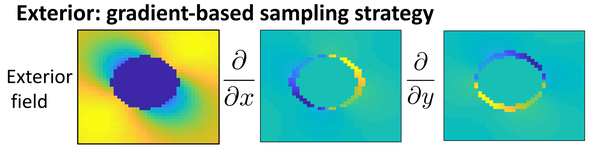
**Lossy compression:** Convolution with impulse-like Greens' function results in a solution which can be sampled at lower rates as distance from the grain increases.
Identifying the regions of interest correctly is important.
Region of interest is sampled at high rates.




**Interior: Identifying contributions from surface stresses**

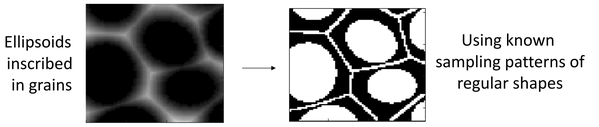



**Exterior: gradient-based sampling strategy**




## Phase II: Plans

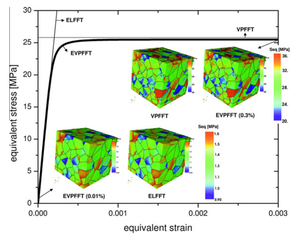
**Thrust 1: Domain decomposition framework for irregular grains**
Irregular grain as a 'packing' of regular shapes (Eg., ellipsoids), for which sampling patterns have been derived

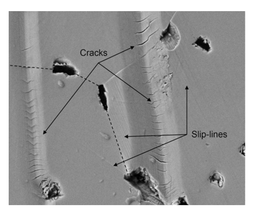



**Thrust 2: Deployment on heterogeneous system with Tesla K80 and Fortran-GPU testing**

Tesla K80
- 24 GB of GDDR5 memory
- 480 GB/s aggregate memory bandwidth

**Thrust 3: Extend to visco-plastic code [2] which includes deformation of crystals and studies cracking and fracture formation**




**Thrust 4: Use FFTX [3], a new framework for building high performance FFT-based applications on exascale machines, for domain-local FFTs.**
**FFTX is backwards compatible to FFTW and has a SPIRAL-based back end for advanced performance optimizations.**

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### References

[1] H. Moulinec and P. Suquet. 1998. A numerical method for computing the over all response of nonlinear composites with complex microstructure. Computer methods in applied mechanics and engineering 157, 1-2 (1998), 69–94.
[2] R. A. Lebensohn. 2001. N-site modeling of a 3D viscoplastic polycrystal using fast Fourier transform. Acta Materialia 49, 14 (2001), 2723–2737.
[3] F. Franchetti et al. 2018. FFTX and SpectralPack: A First Look. PFFT Workshop, 2018.