GPU-accelerated Bloch wave calculation for quantitative structure factor determination

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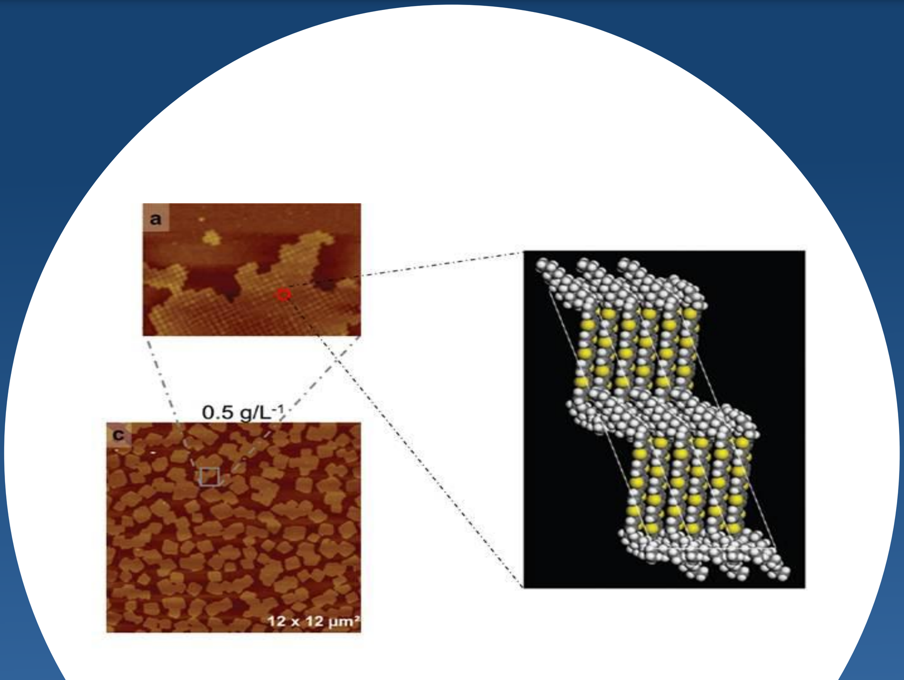
Motivation



M. Defaux et al., Advanced Materials 24 (2012) 973–978

analysis of the atomic structure of very small volumes

- thin (nano crystals are not 150nm thick)
- light elements (organic)
- large unit cell
  - organic thin films for OLEDs, OFETs
  - 2D crystals 10-30nm thick and big unit cell

Dynamical electron diffraction simulation using the Bloch waves

the propagation of electrons in matrix notation

$$\psi(t) = \mathbf{S}(t)\psi(0)$$

S is the scattering matrix

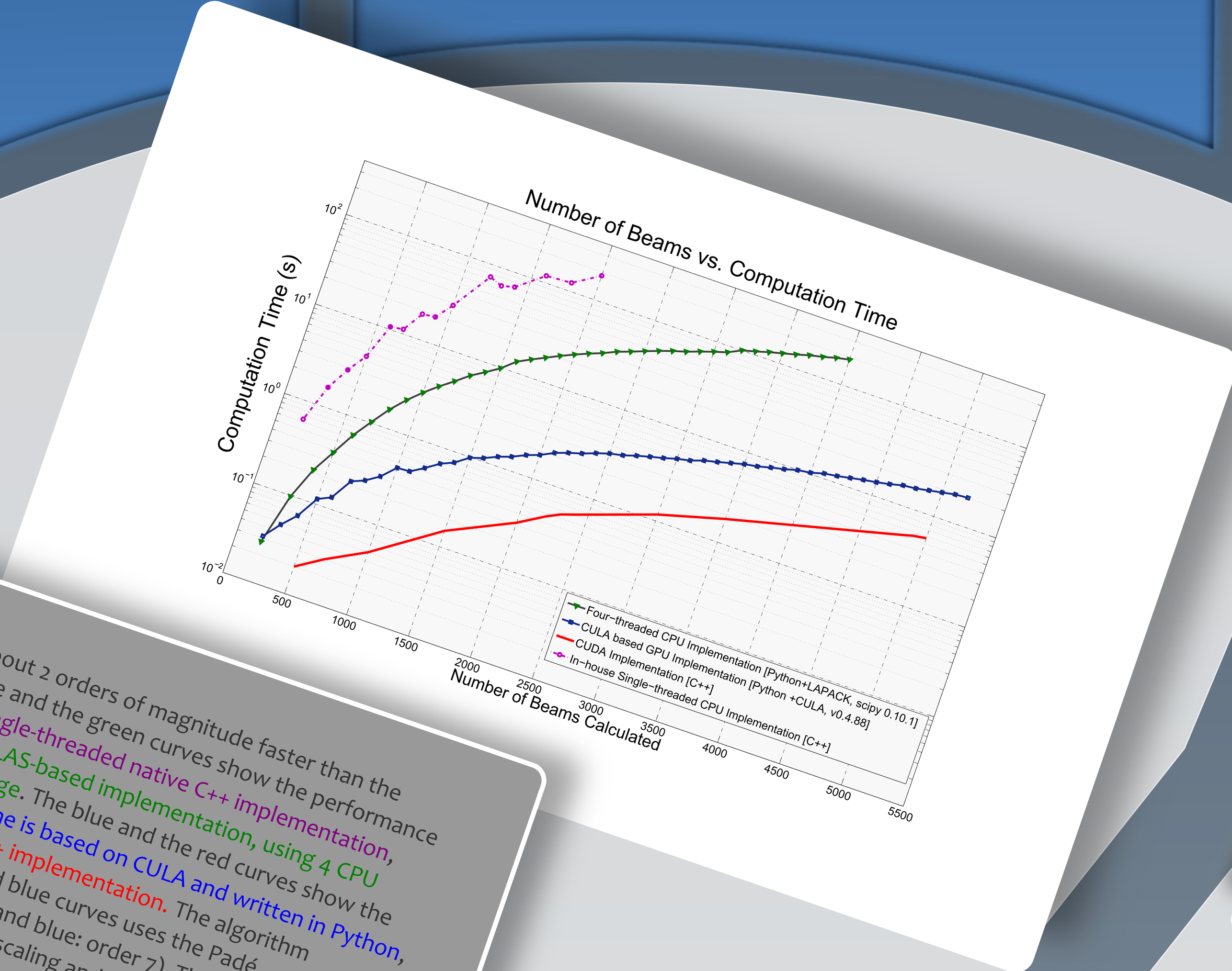
$$\mathbf{S} = e^{i\pi\lambda t\mathbf{A}}$$

A is the structure factor matrix

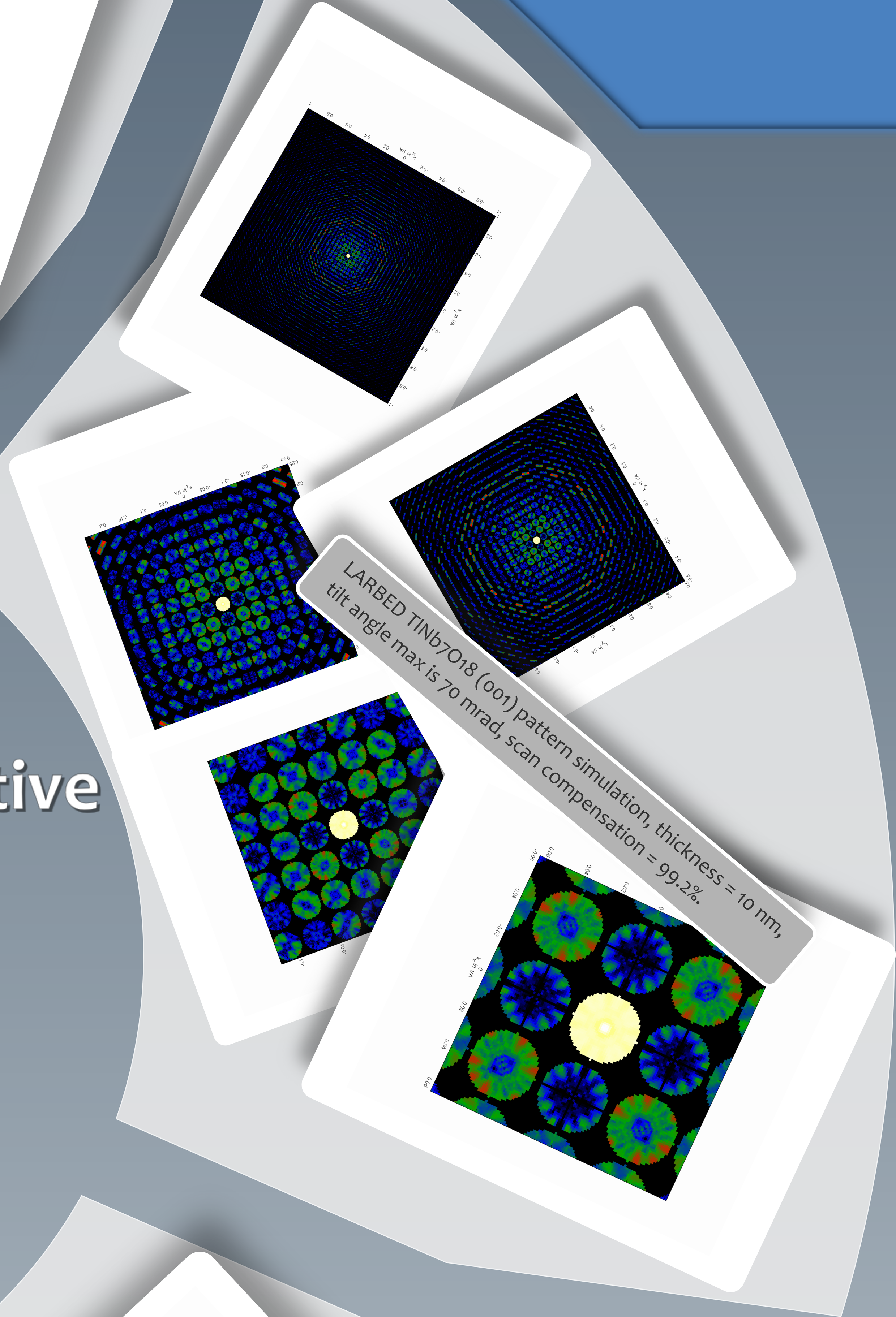
$$A = \begin{pmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \iddots \\ \cdots & U_0-(k_t+h)^2 & U_{h-g} & U_h & U_{h+g} & U_{h+h} & \cdots \\ \cdots & U_{g-h} & U_0-(k_t+g)^2 & U_g & U_{g+g} & U_{g+h} & \cdots \\ \cdots & U_{-h} & U_{-g} & U_0-k_t^2 & U_g & U_h & \cdots \\ \cdots & U_{-g-h} & U_{-g-g} & U_{-g} & U_0-(k_t-g)^2 & U_{-g+h} & \cdots \\ \cdots & U_{-h-h} & U_{-h-g} & U_{-h} & U_{-h+g} & U_0-(k_t-h)^2 & \cdots \\ \iddots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

the intensity of the spots in the diffraction are squared moduli of the central column of S

$$I_{m,n} = |S_{m,n}|^2 = [e^{i\pi\lambda t\mathbf{A}}]_{m,n}[e^{i\pi\lambda t\mathbf{A}}]^*_{m,n}$$

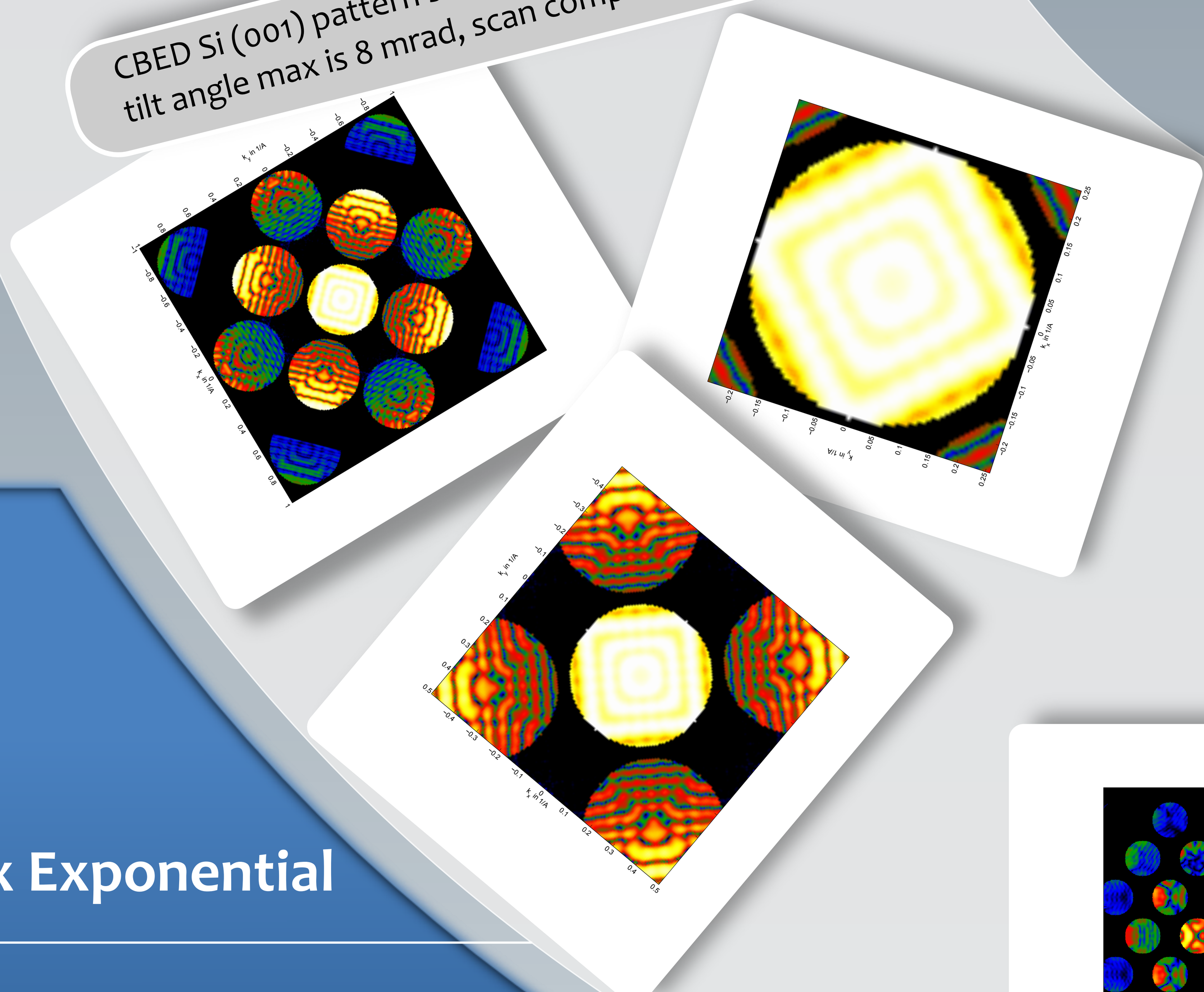


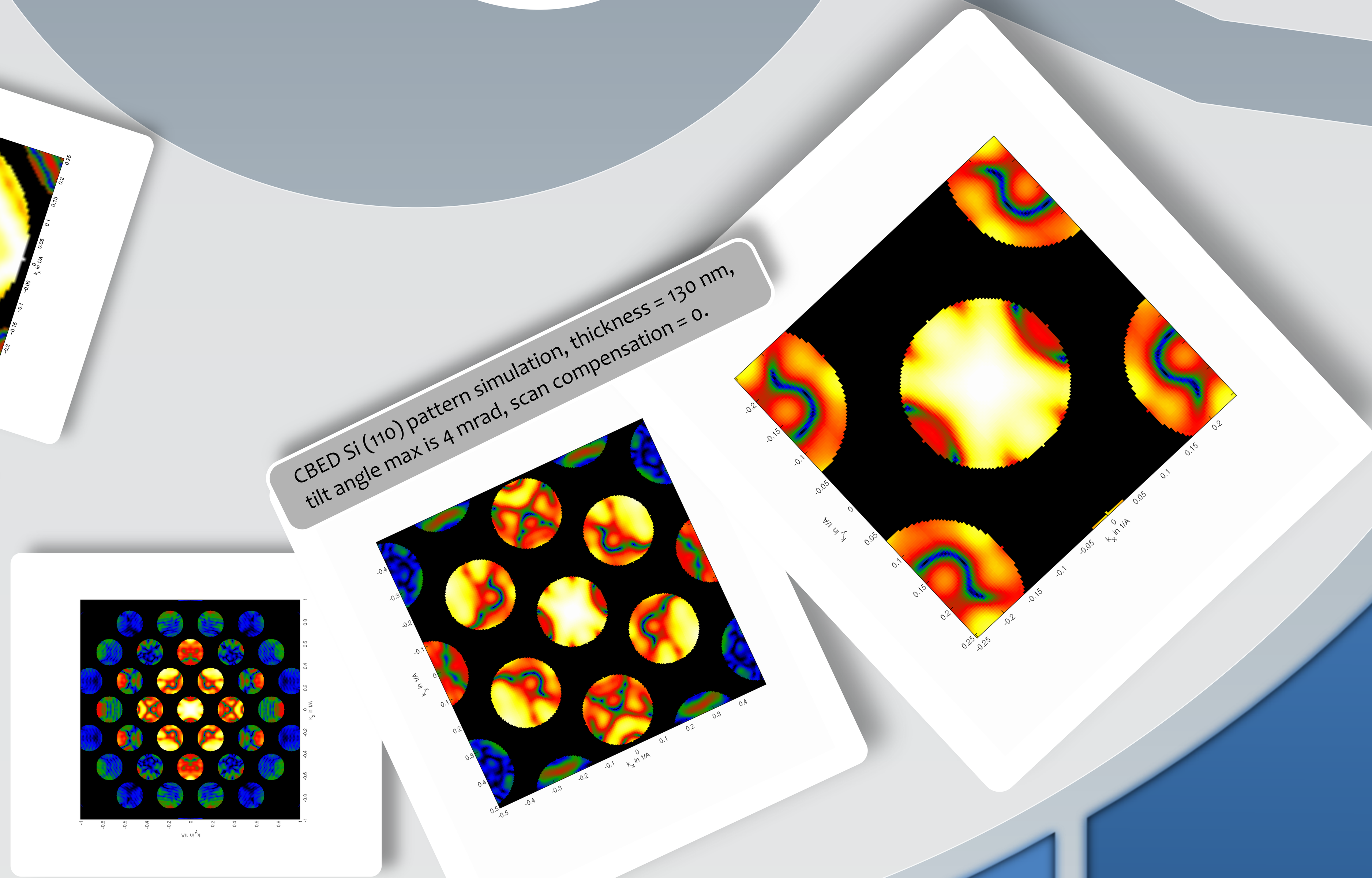
The GPU-based CUDA code is about 2 orders of magnitude faster than the parallelized CPU code. The purple and the green curves show the performance on the CPU: the purple one is a single-threaded native C++ implementation, while the green one is a LAPACK/BLAS-based implementation, using 4 CPU threads and the SciPy Python package. The blue and the red curves show the performance on the GPU: the blue one is based on CULA and written in Python, while the red one is a native CUDA C++ implementation. The algorithm corresponding to the purple, green and blue curves uses the Padé approximation (purple: order 14, green and blue: order 7). The algorithm corresponding to the red curve uses the scaling and squaring method.



LARBED TiNb7O18 (001) pattern simulation, thickness = 10 nm, tilt angle max is 70 mrad, scan compensation = 99.2%.

CBED Si (001) pattern simulation, thickness = 130 nm, tilt angle max is 8 mrad, scan compensation = 0.





CBED Si (110) pattern simulation, thickness = 130 nm, tilt angle max is 4 mrad, scan compensation = 0.

Matrix Exponential

Scaling & Squaring with Power Series

- $B \leftarrow \dfrac{A}{2^s}$ so $||B||_\infty \simeq 1$
- $e^B = I + B + \dfrac{B^2}{2!} + \dfrac{B^3}{3!} + \dfrac{B^4}{4!} + \dfrac{B^5}{5!} + \ldots$
- $e^A \simeq \{e^B\}^{\{2^s\}}$

Polynomial Truncation

$$e^B \simeq I + B + \frac{B^2}{2!} + \frac{B^3}{3!} + \frac{B^4}{4!} + \frac{B^5}{5!} + \frac{B^6}{6!} + \frac{B^7}{7!} + \frac{B^8}{8!} + \frac{B^9}{9!}$$

8 matrix-matrix multiplications

$$e^B \simeq (a_0I+a_1B+a_2B^2+a_3B^3)\,(b_0I+b_1B+b_2B^2+b_3B^3)\,(c_0I+c_1B+c_2B^2+c_3B^3)$$

4 matrix-matrix multiplications

or
a = { 1.04769359793033, 0.136216585231228, 0.175032858463863, 0.00019558817717526 };

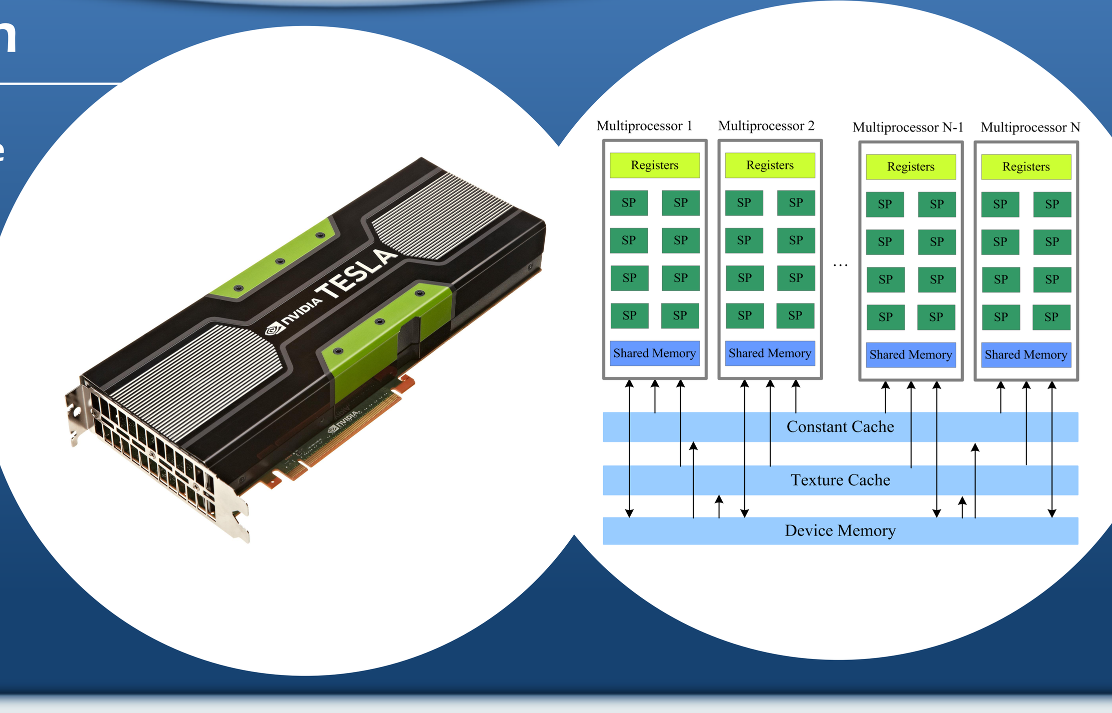
CUDA Acceleration

Nvidia Tesla K20C Performance

- Single Precision Performance 2.04 Tflops/s
- Double Precision Performance 1.16 Tflops/s

Intel(R) Xeon(R) CPU W3550

- Single Precision Performance 0.02 Tflop/s



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