Modeling of Graphene Membrane Rupture with Density Functional Tight Binding

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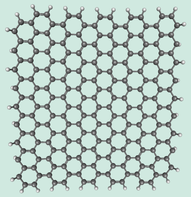
Abstract

Density Functional Tight Binding (DFTB) is being used to find the cause of the catastrophic rupture of a graphene membrane under the effect of an electric field. Efforts are also being made to increase the computational efficiency of the program by replacing LAPACK calls with ScaLAPACK calls.

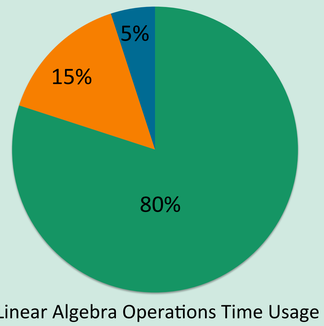


Introduction

DFTB+ is being used to find out why a graphene membrane is rupturing under an electric field. When an electric field of 3 V/nm is applied to a graphene sheet suspended in a 1 M KCl solution, the membrane ruptures catastrophically, sometimes ripping completely in half.

Carbons	Hydrogens	Corners	Flat or Warped
218	40	Free	Flat
			Warped
		Frozen	Flat
			Warped
	58	Free	Flat
			Warped
		Frozen	Flat
			Warped
508	62	Free	Flat
			Warped
		Frozen	Flat
			Warped
	90	Free	Flat
			Warped
		Frozen	Flat
			Warped

Several different variations of graphene membranes are being tested under varying conditions using molecular dynamics (MD) simulations. These can be seen in the above table.

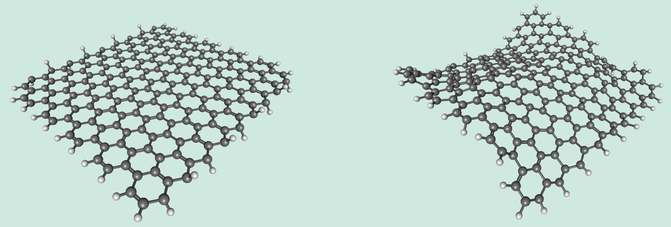


The most computationally expensive component of DFTB code is its linear algebra operationssuch as matrix-matrix multiplication, Cholesky factorizations, and dialgonalizations.

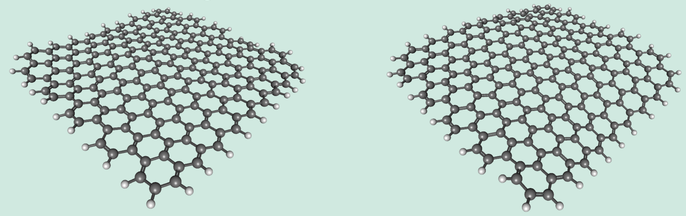
As conditions for the calculations become more complex the time also increases.

Simulations

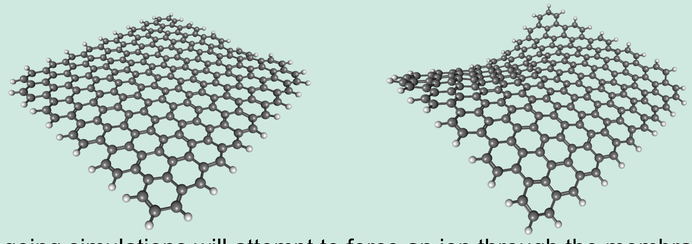
To simulate a 3 V/nm electric field in DFTB+, a 15 eV point charge is placed 100 Å away, along a vector normal to the membrane. A -15 eV point charge mirrors the first on the other side of the membrane. Below are the flat and warped membranes input into DFTB.



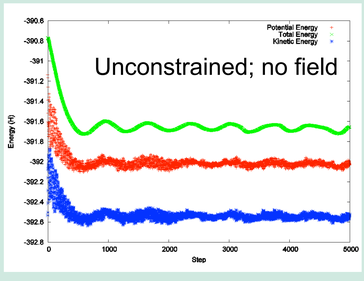
Below are the output geometries of a 5000-step MD simulation.



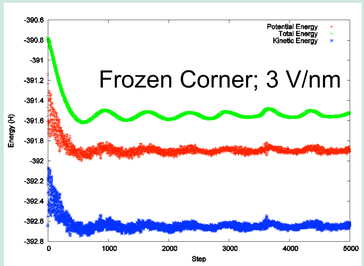
Below are the output geometries with the corners frozen.

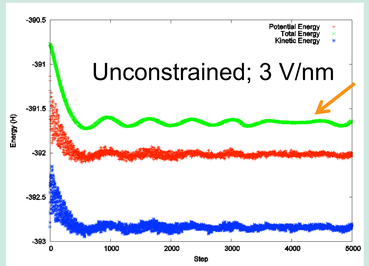


Ongoing simulations will attempt to force an ion through the membrane.



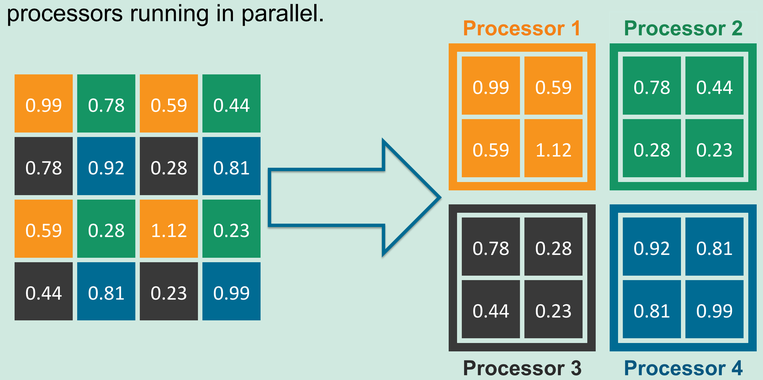
Changes in the membranes' energies were recorded during MD simulations. Notice the flattened region in the unconstrained field run. The unconstrained warped membrane behaved similarly. No other runs exhibit this region.





LAPACK to ScaLAPACK

Current DFTB code utilizes LAPACK (Linear Algebra Package) function calls to perform its linear algebra operations such as matrix-matrix multiplication, Cholesky factorizations, and dialgonalizations. By replacing the LAPACK routines with ScaLAPACK (Scalable LAPACK) routines, the calculation speed can be improved. ScaLAPACK has the advantage of distributing the matrix data in a block-cyclic fashion to processors running in parallel.



The distributed memory will allow for faster calculations as well as the ability to increase the problem size and complexity.

LAPACK	Time (s)	ScaLAPACK	16 Processes Time (s)	25 Processes Time (s)
DGEMM	40.0	PDGEMM	38.2	23.5
DPOTRF	6.7	PDPOTRF	7.4	5.0
DPOTRI	25.1	PDPOTRI	2.30	21.1
DSYEV	365.2	PDSYEV	259.2	190.4
DSYEVD	254.6*	PDSYEVD	215.5	89.6
DSYGVD	333.1	PDSYGVX	0.0	0.0

*Calculation performed on Darter

A comparison of operations on a 16834 X 16834 matrix run on Beacon show ScaLAPACK calls exhibit significantly faster computational speed.

Acknowledgements

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References

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