ViennaSHE: A Semiconductor Device Simulator based on the Spherical Harmonics Expansion Method

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Applied Mathematics and Simulation for Semiconductors
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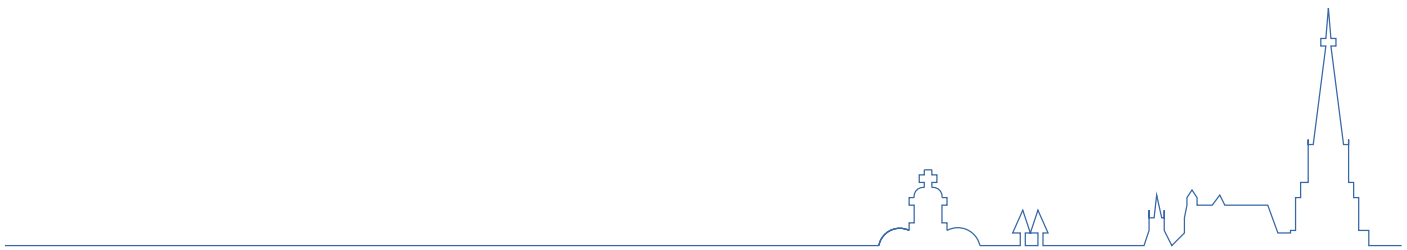
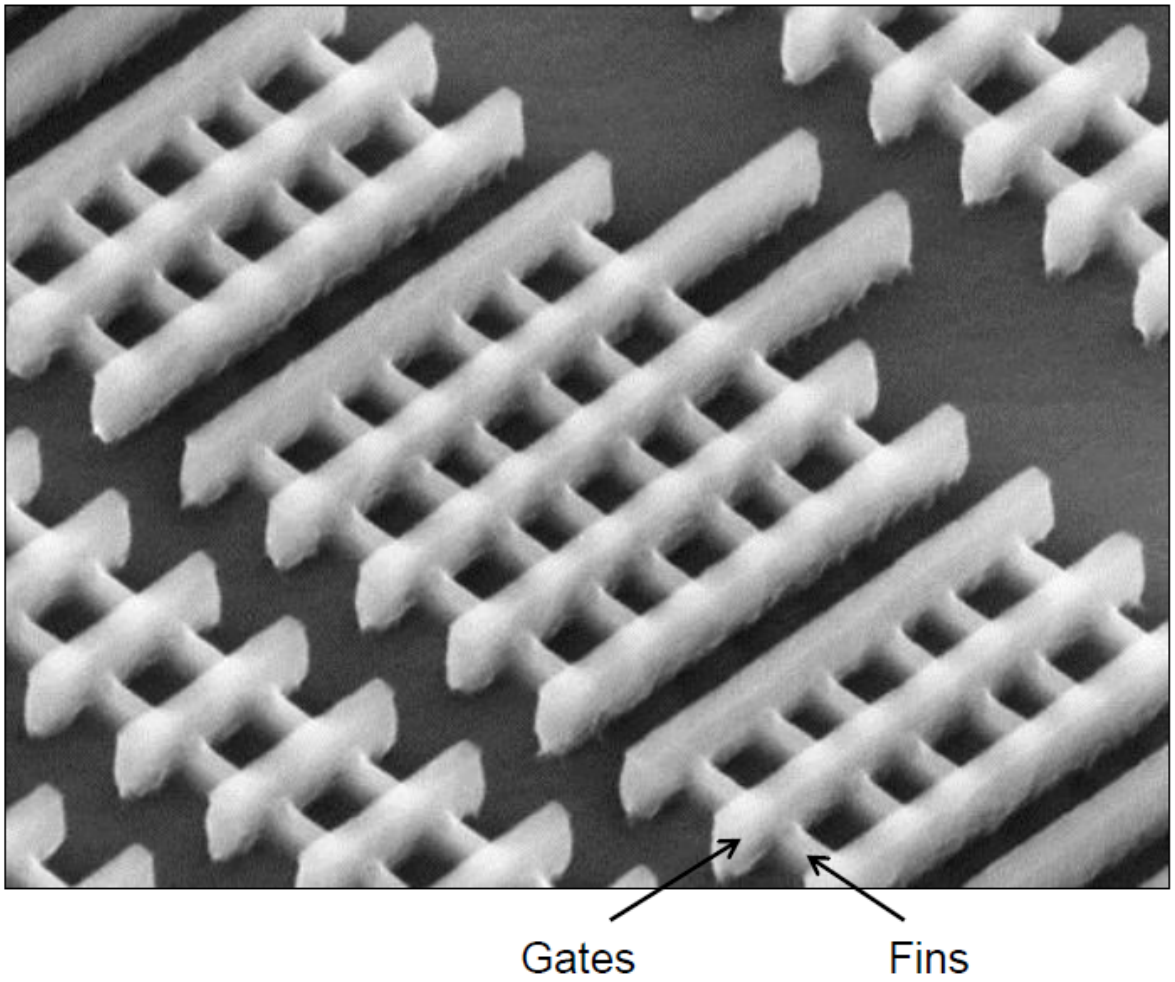
Contents

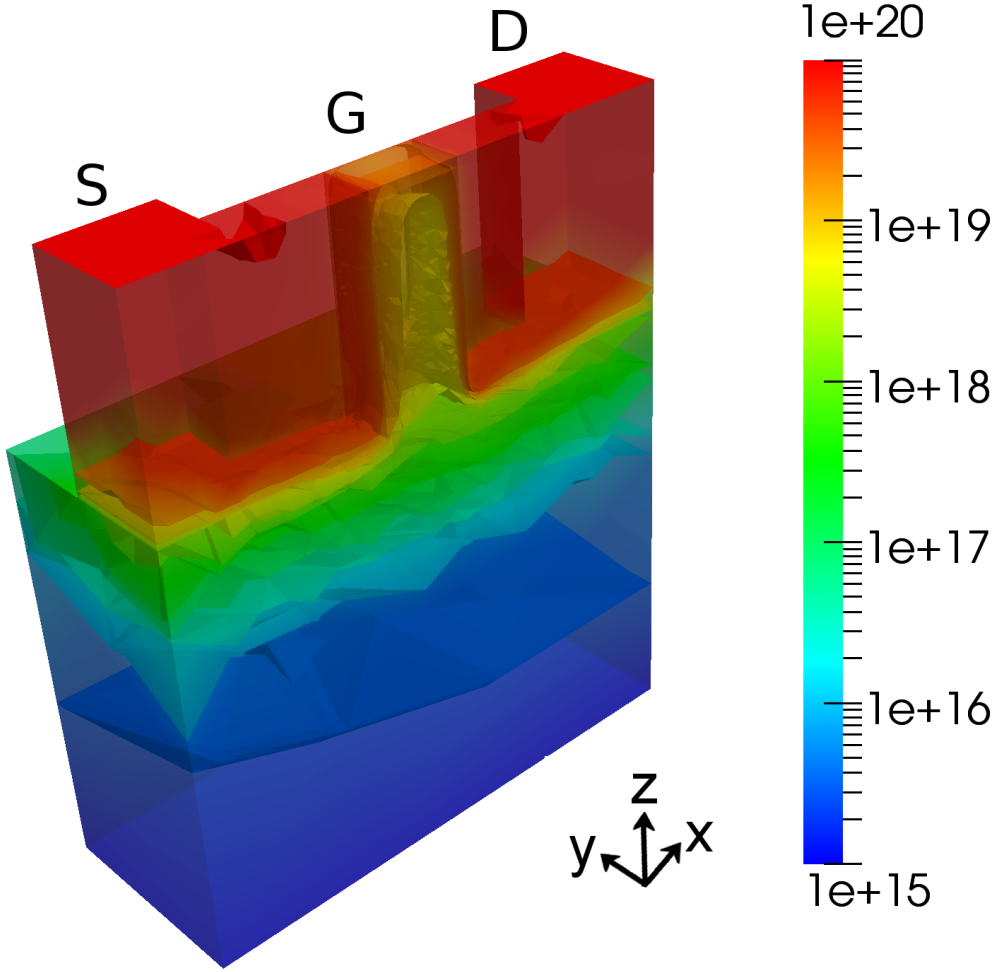


Semiconductor Devices in 3D: FinFET

Intel Trigate transistors

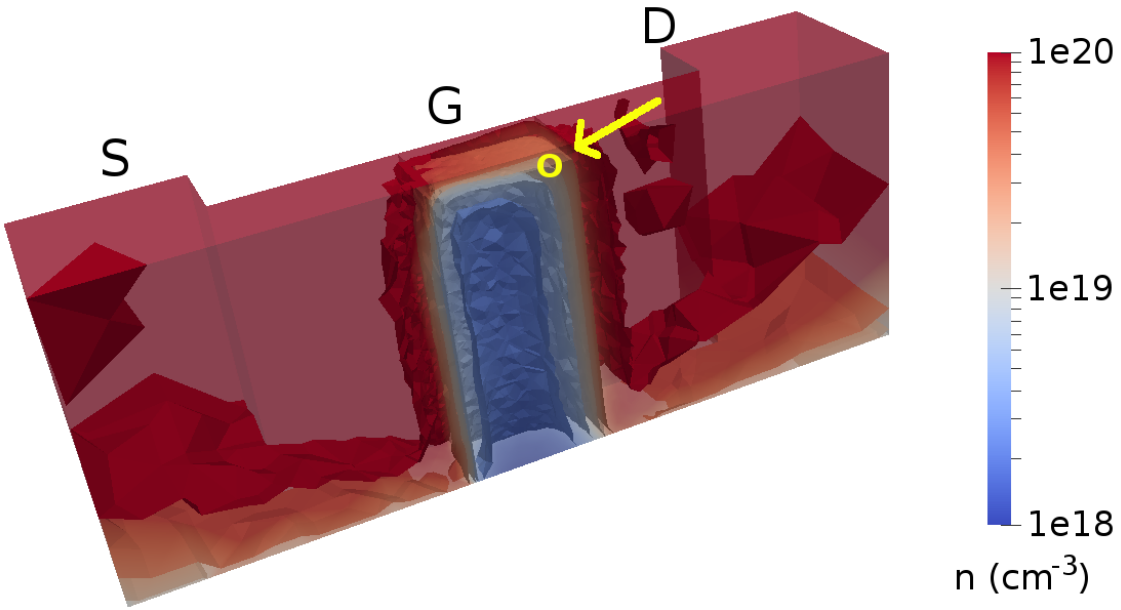


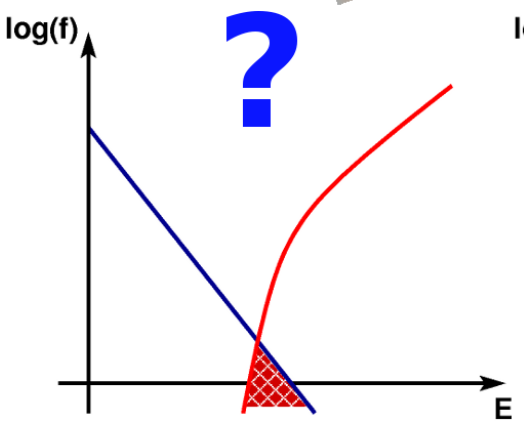
Semiconductor Devices in 3D: FinFET

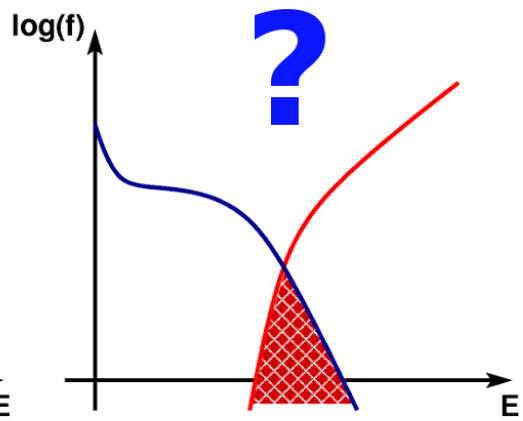


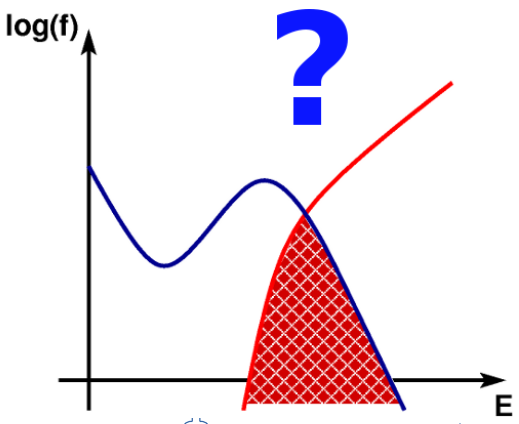
Electron Energy Distribution?

Distribution of electrons with respect to energy at x?









Electron Energy Distribution?

Macroscopic Transport Models

Invalid in deca-nanometer regime

“Fitting” only treats the symptoms, not the cause

Only averaged quantities of the carrier ensemble modeled

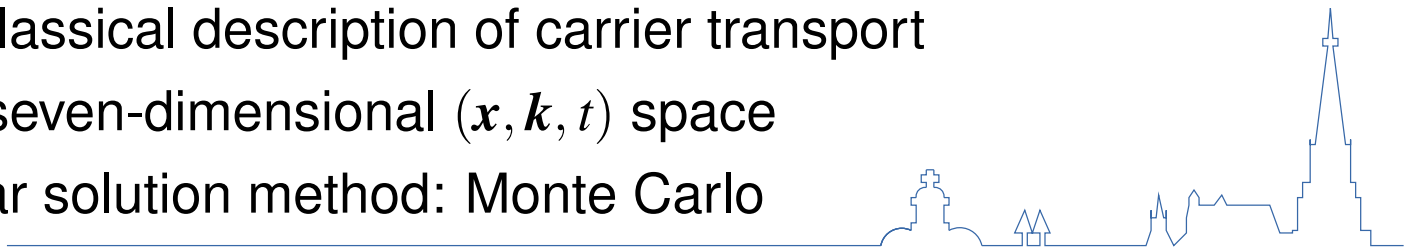
Boltzmann Transport Equation (BTE)

$$\frac{\partial f}{\partial t} + \boldsymbol{v}(\boldsymbol{k}) \cdot \nabla_{\boldsymbol{x}} f + \boldsymbol{F}(\boldsymbol{x}) \cdot \nabla_{\boldsymbol{k}} f = Q\{f\}$$

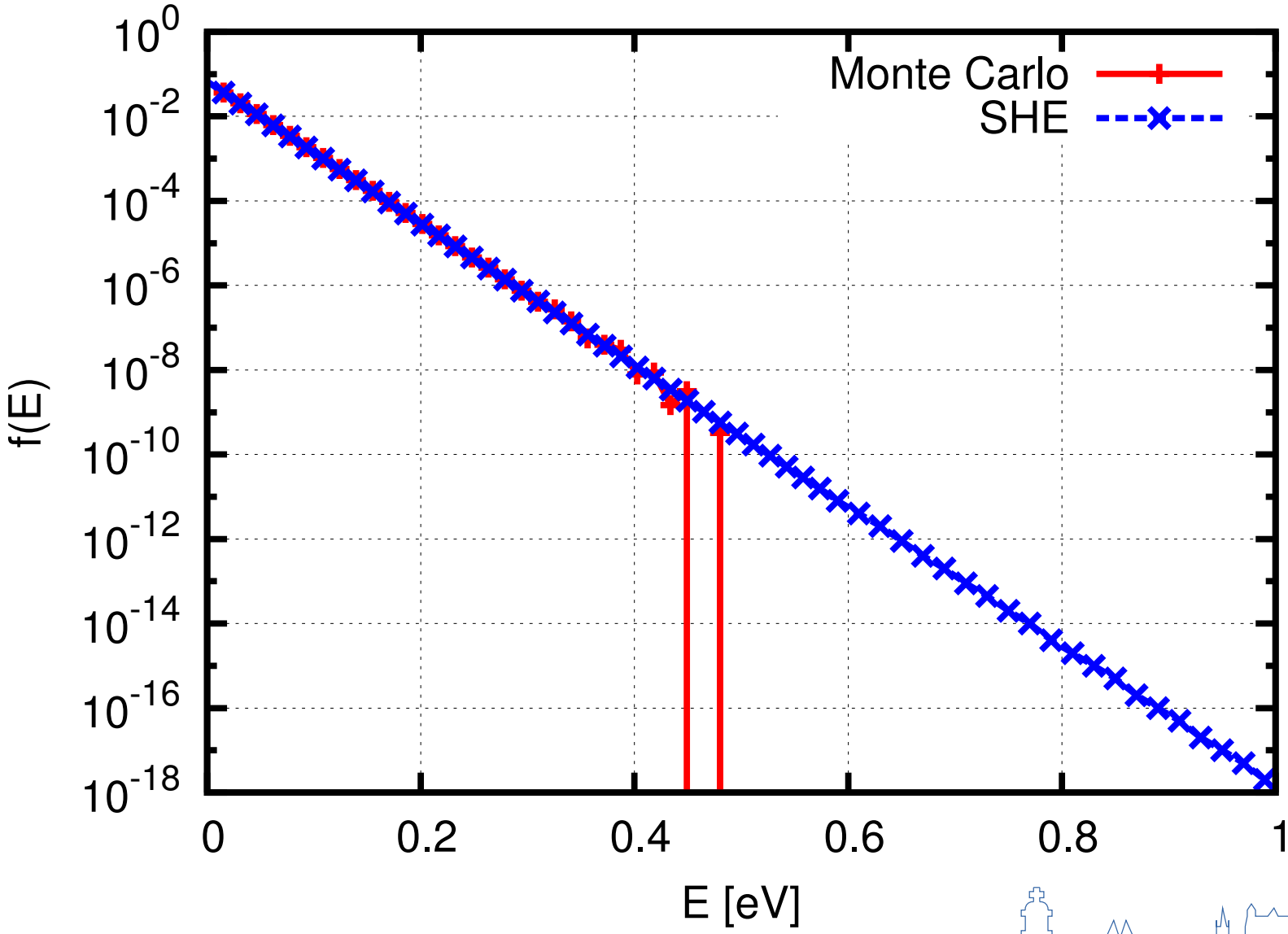
Best semi-classical description of carrier transport

Posed in a seven-dimensional $(\boldsymbol{x}, \boldsymbol{k}, t)$ space

Most popular solution method: Monte Carlo



Electron Energy Distribution?



Spherical Harmonics Expansion Method

Spherical Symmetries

Maxwell distribution of carriers at equilibrium

Dispersion relation (Herring-Vogt transform, approx.)

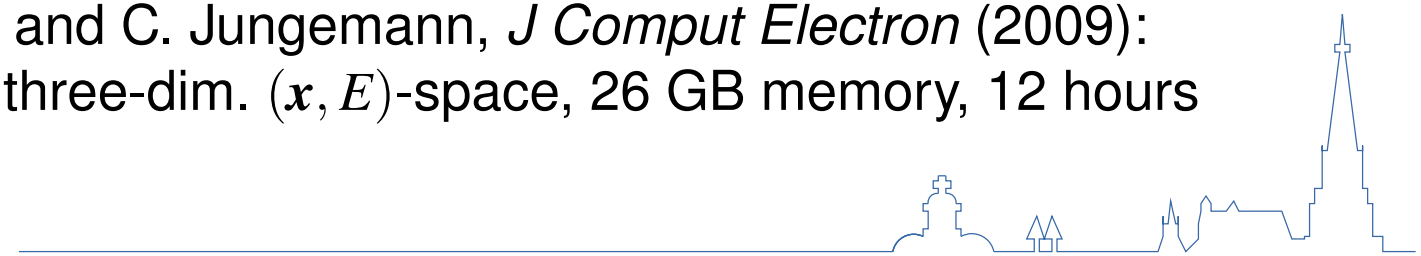
Spherical Harmonics Expansion (SHE)

$$f(\boldsymbol{x},\boldsymbol{k},t) \simeq \sum_{l=0}^{L} \sum_{m=-l}^{l} f_{l,m}(\boldsymbol{x},E,t) Y_{l,m}(\theta,\varphi)$$

New unknowns: $f_{l,m}(\boldsymbol{x},E,t)$

Solution in five-dimensional $(\boldsymbol{x},E,t)$-space

S.-M. Hong and C. Jungemann, *J Comput Electron* (2009):
Fifth-order, three-dim. $(\boldsymbol{x},E)$-space, 26 GB memory, 12 hours



Unstructured Grids

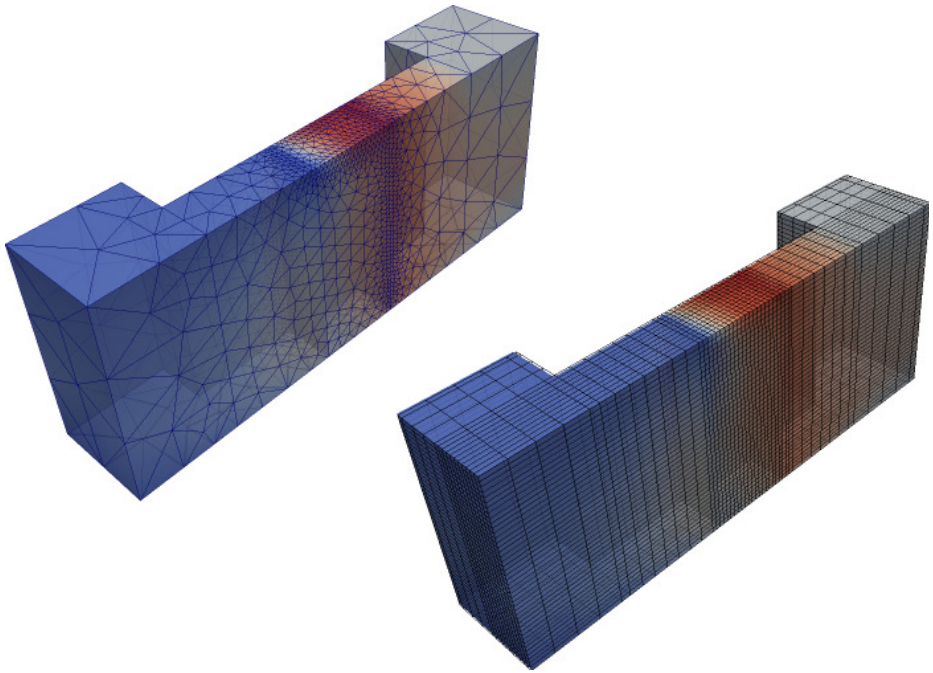
State-of-the-art in modern TCAD

Only structured grids in publications on higher-order SHE in 2D

[S.-M. Hong and C. Jungemann (2008), S.-M. Hong and C. Jungemann (2009)]

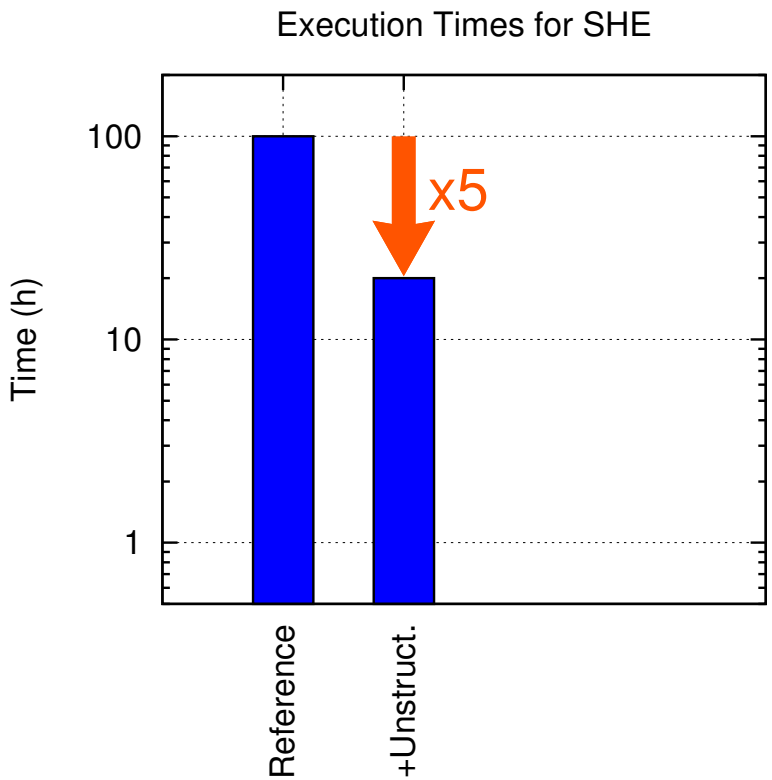
Extension of discretization proposed by Hong and Jungemann

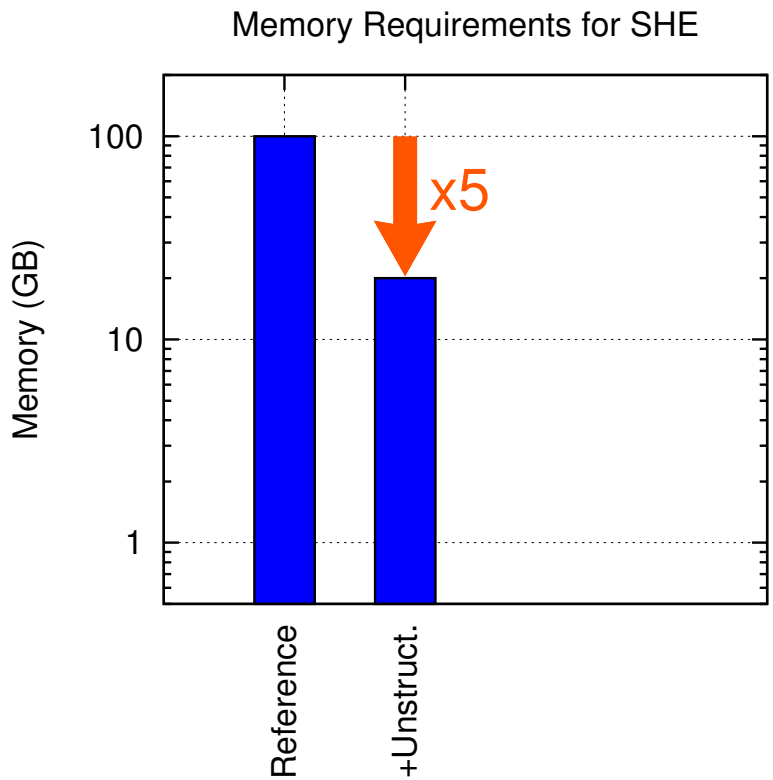
4838 nodes



27456 nodes

Summary


Execution Times for SHE
Time (h)
100
10
1
x5
Reference
+Unstruct.


Memory Requirements for SHE
Memory (GB)
100
10
1
x5
Reference
+Unstruct.

Adaptive Variable-Order SHE

Spherical Harmonics Expansion

$$f(\boldsymbol{x},\boldsymbol{k},t) \simeq \sum_{l=0}^{L} \sum_{m=-l}^{l} f_{l,m}(\boldsymbol{x},E,t) Y_{l,m}(\theta,\varphi)$$

$(L+1)^2$ unknown functions $f_{l,m}(\boldsymbol{x},E,t)$

$L=0$ sufficient in equilibrium

Higher-order expansions in active regions

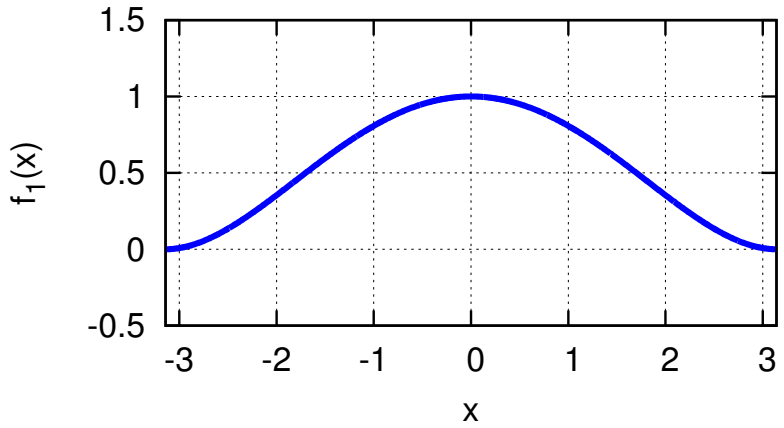
Therefore: Variable-order SHE:

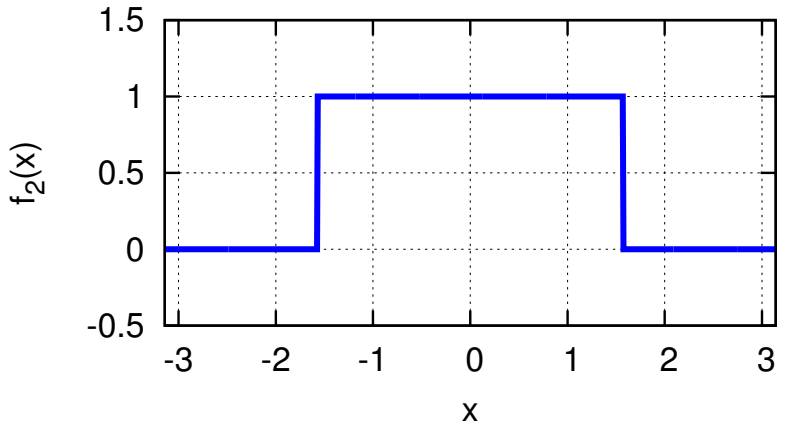
$$f(\boldsymbol{x}_i,\boldsymbol{k}_n,t) \simeq \sum_{l=0}^{L(\boldsymbol{x}_i,E_n)} \sum_{m=-l}^{l} f_{l,m}(\boldsymbol{x}_i,E_n,t) Y_{l,m}(\theta,\varphi)$$

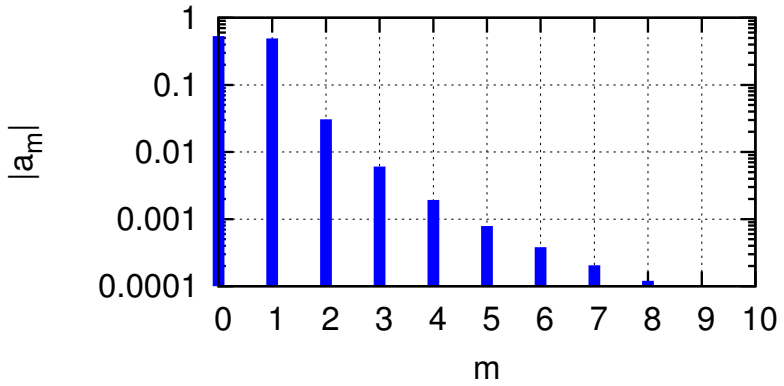
How to choose $L(\boldsymbol{x}_i,E_n)$ in the simulation domain?

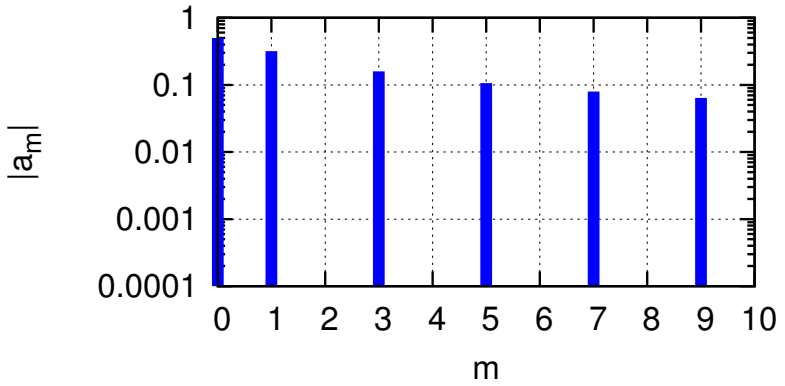
Adaptive Variable-Order SHE

Motivation from Fourier series







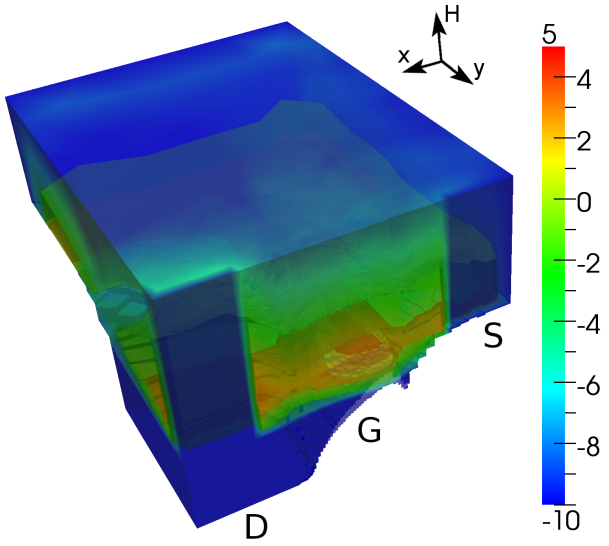


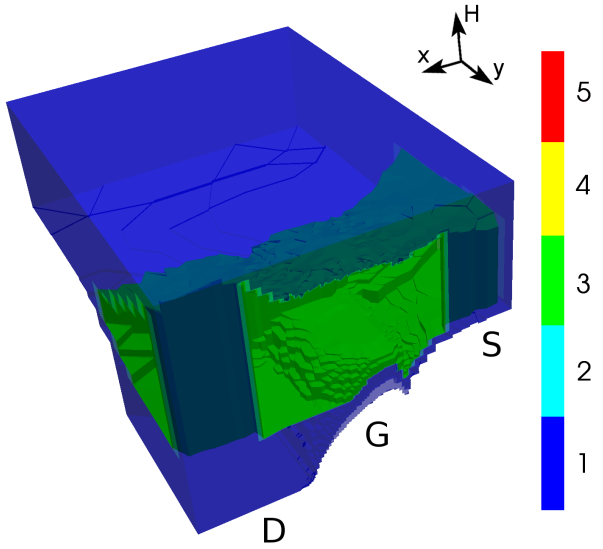
Adaptive Variable-Order SHE

Error indicator:

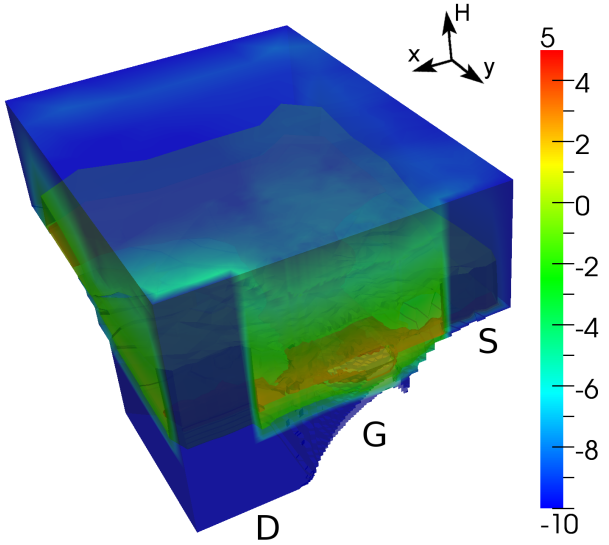
Expansion order:

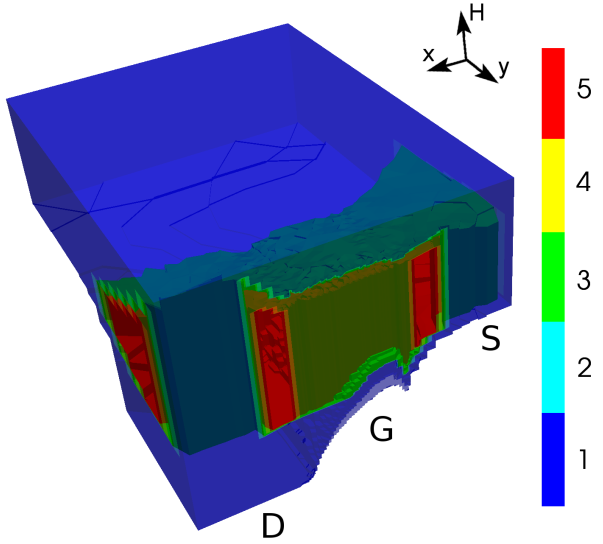
$L = 1$



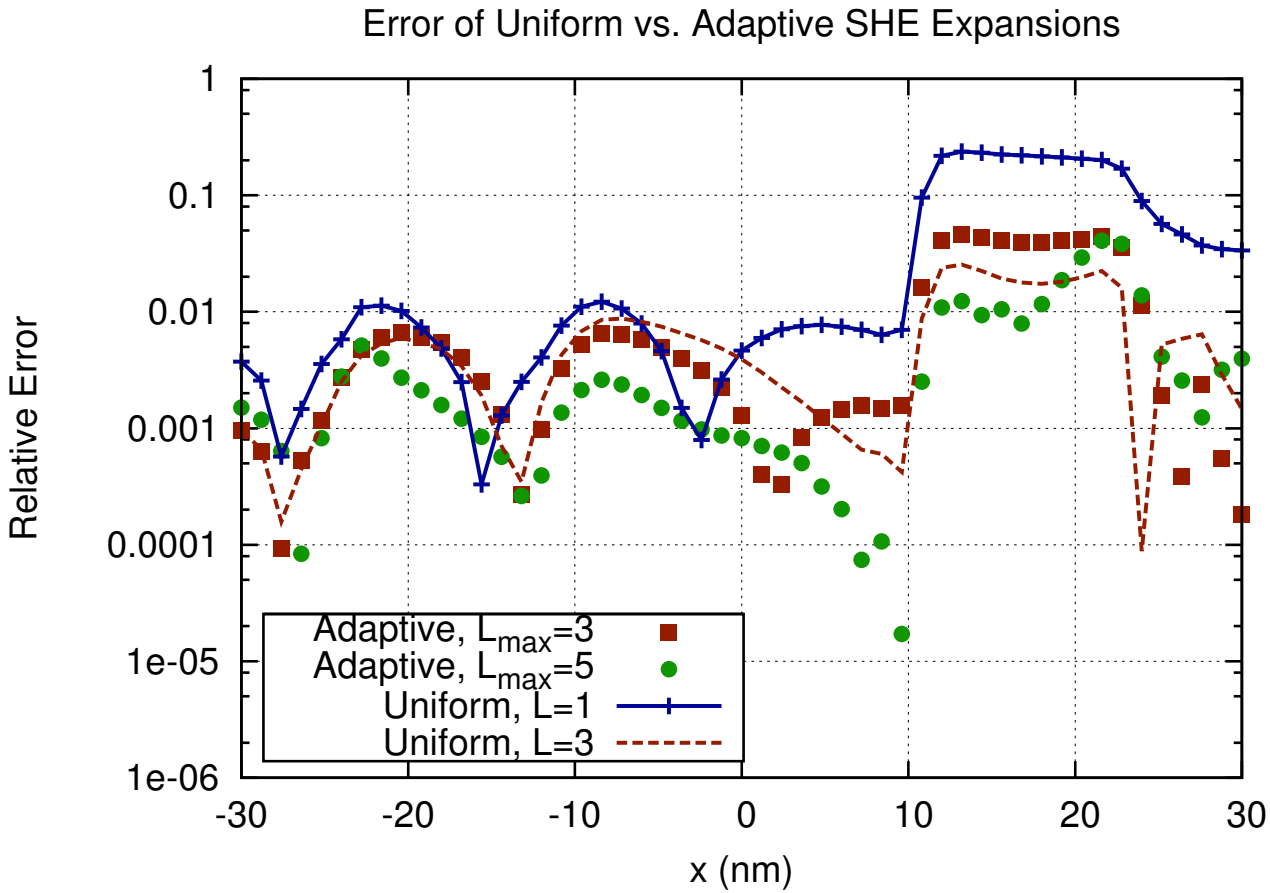


$L = 3$





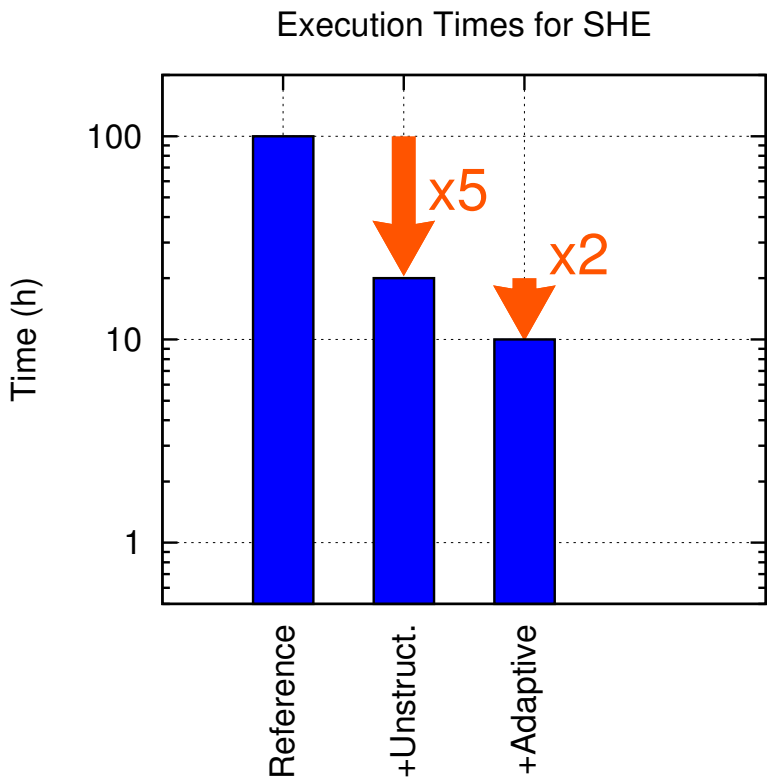
Adaptive Variable-Order SHE

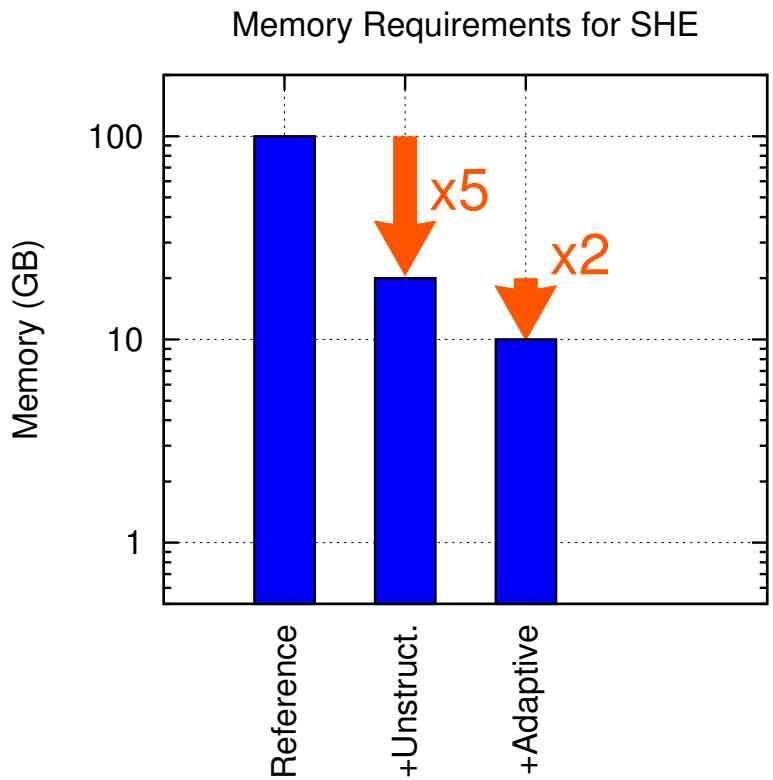


$L = 3$: **306 261** instead of **476 061** unknowns (factor **1.5**)

$L = 5$: **606 671** instead of **1 146 120** unknowns (factor **1.9**)

Summary


Execution Times for SHE
Time (h)
100
10
1
x5
x2
Reference
+Unstruct.
+Adaptive

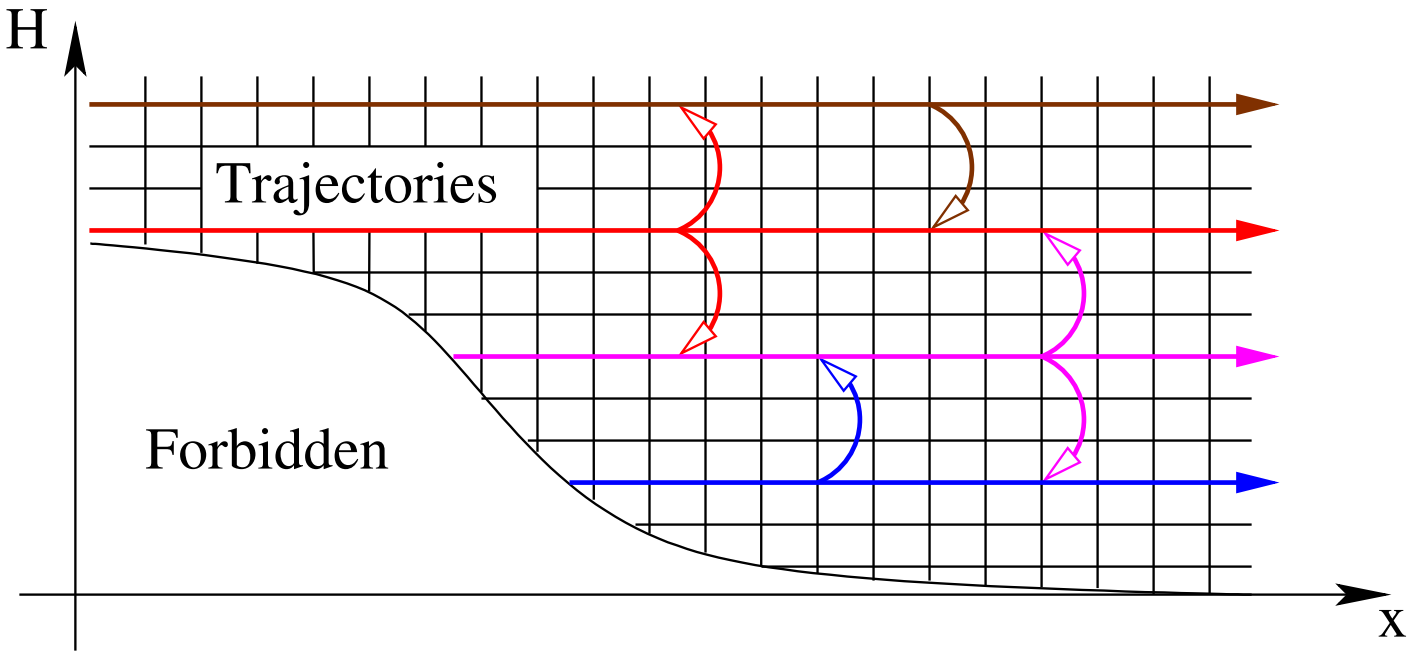

Memory Requirements for SHE
Memory (GB)
100
10
1
x5
x2
Reference
+Unstruct.
+Adaptive

Parallelization

Preconditioner for Iterative Linear Solvers

No fast general-purpose parallel preconditioner available

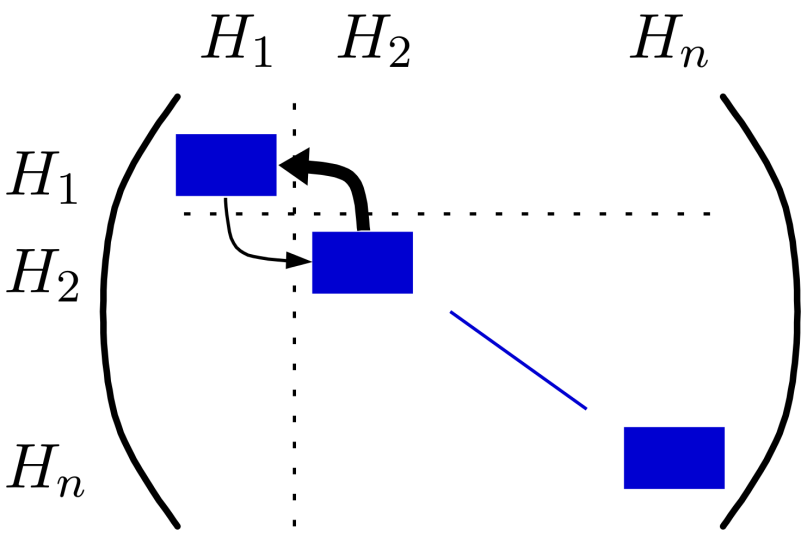
Physics-based parallel block preconditioner developed

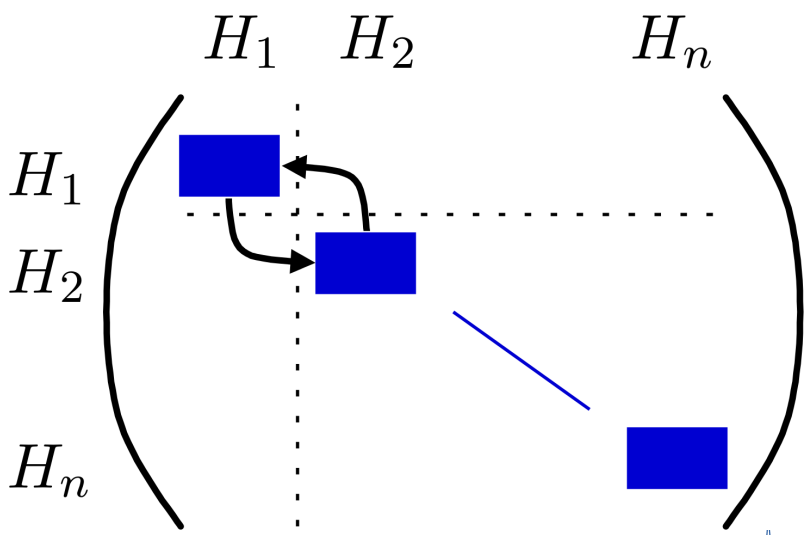


Scaling of Solution Variables

Exponential decay with energy: $f(E_i) \sim \exp(-\frac{E_i}{k_B T})$

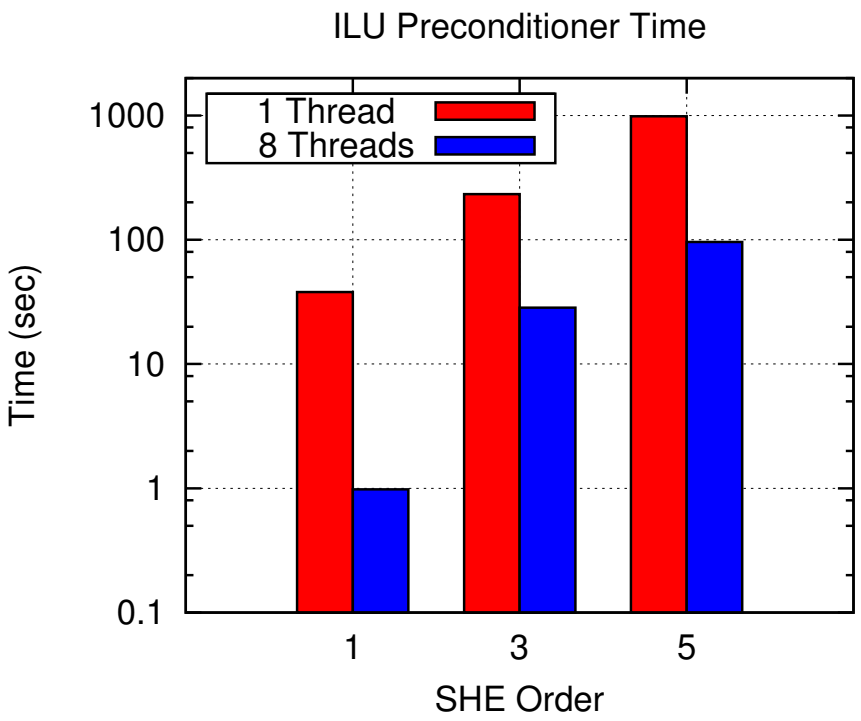
Rescale unknowns: $\tilde{f}(E_i) = \exp(\frac{E_i}{k_B T}) f(E_i)$

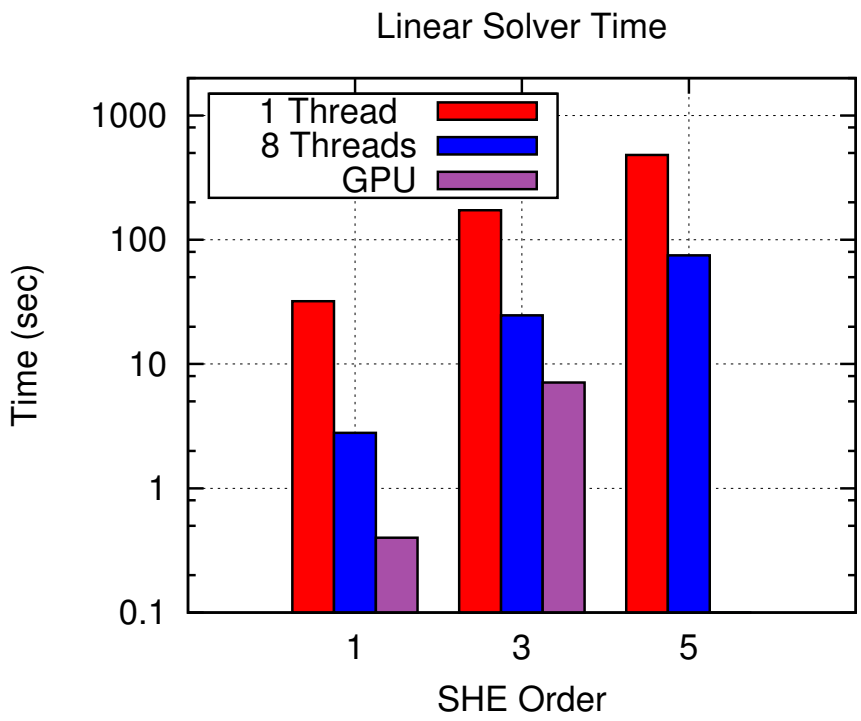




Parallelization

Benchmark results for a FinFET (INTEL Core i7 960, NVIDIA GTX 580)





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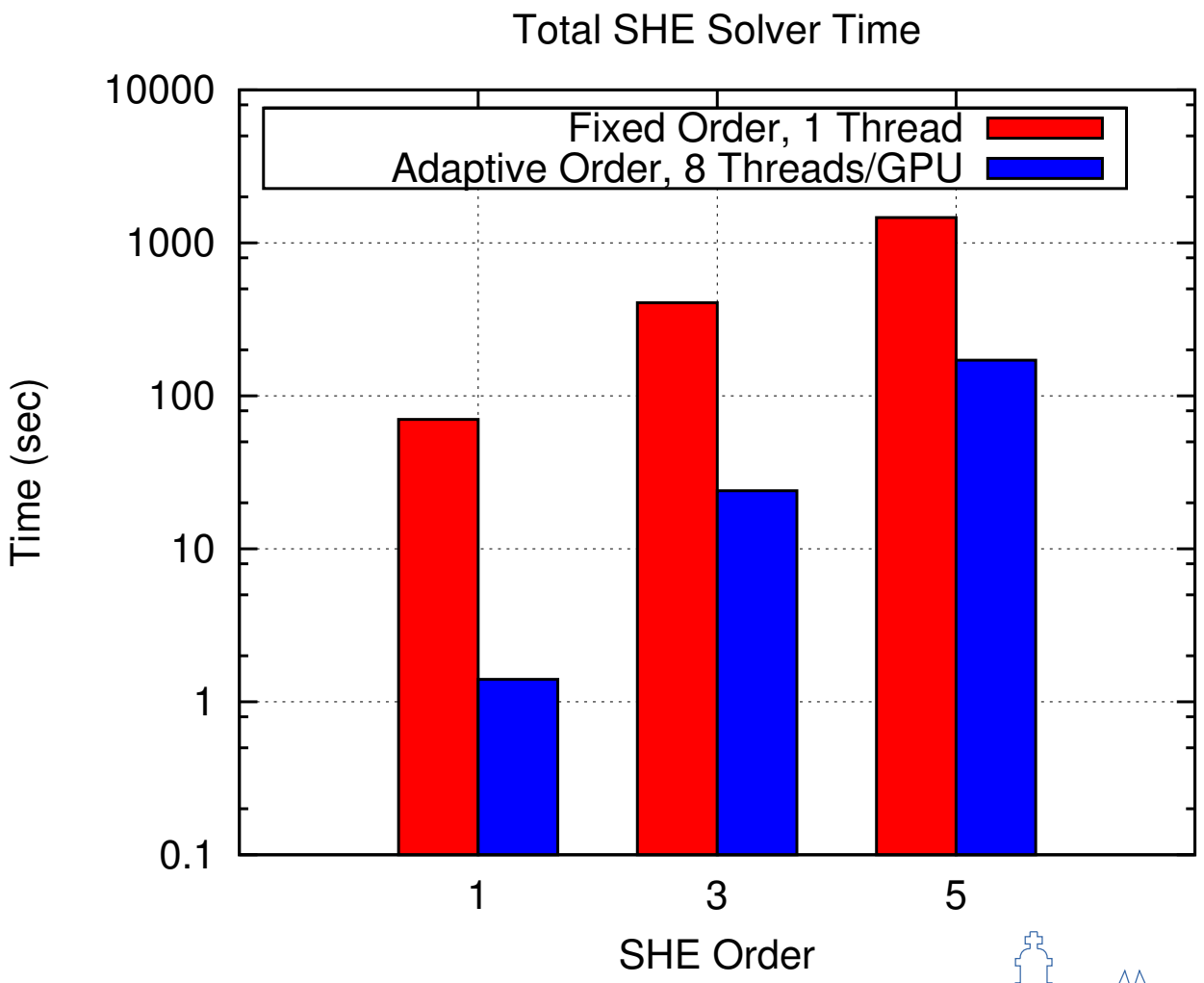
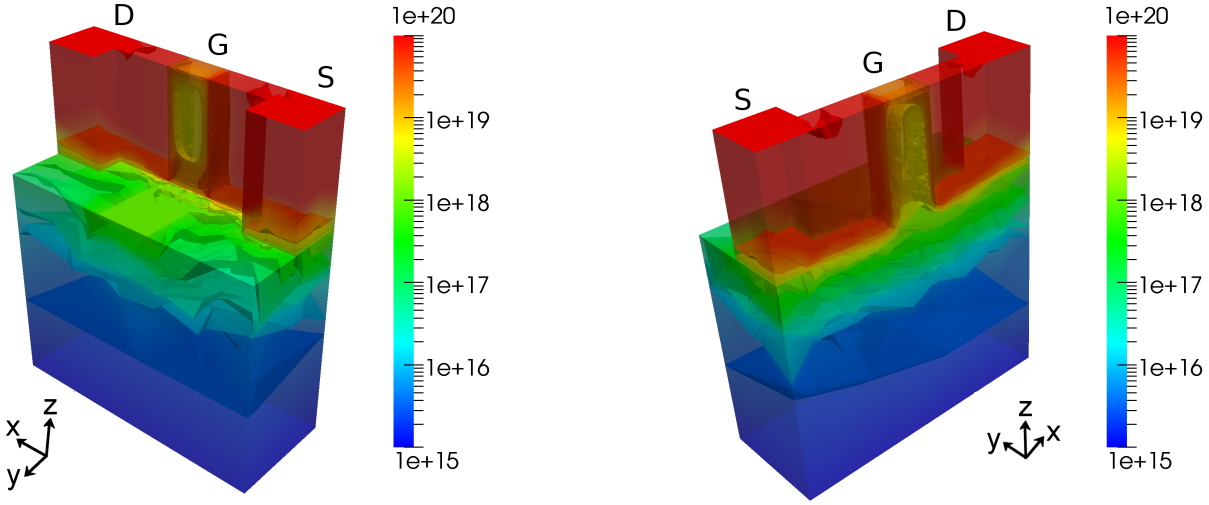
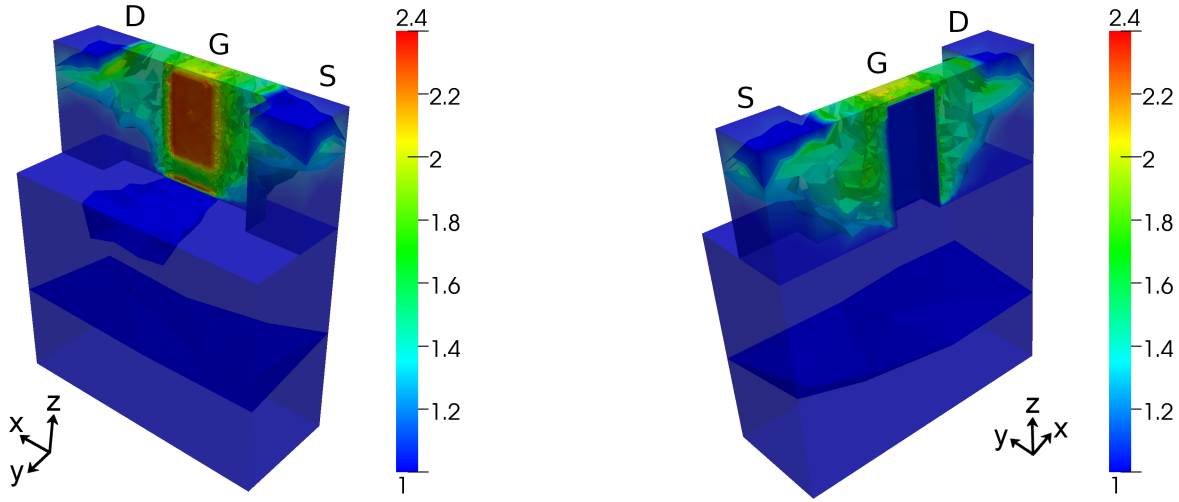


Results

Electron Concentration (cm^{-3})

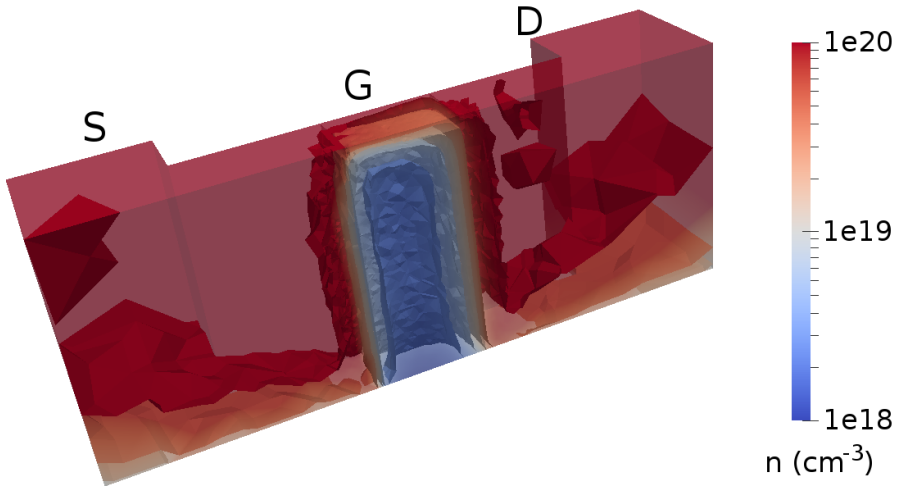


Avg. Expansion Order

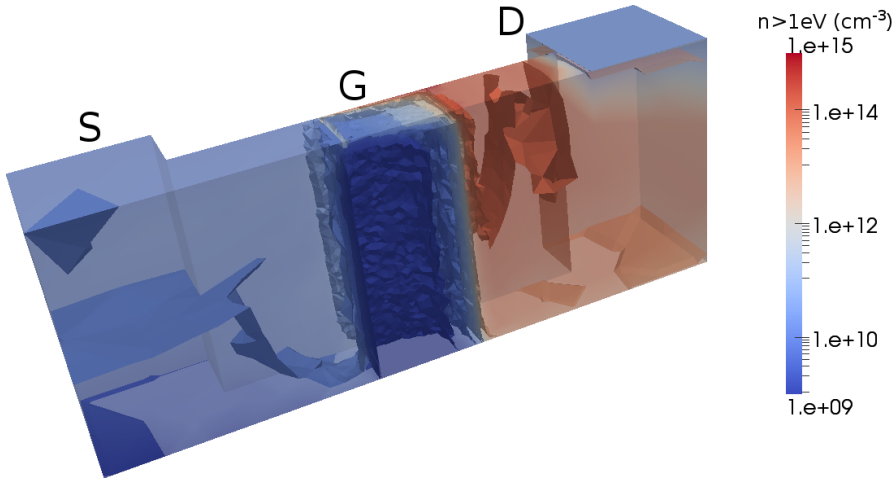


Results

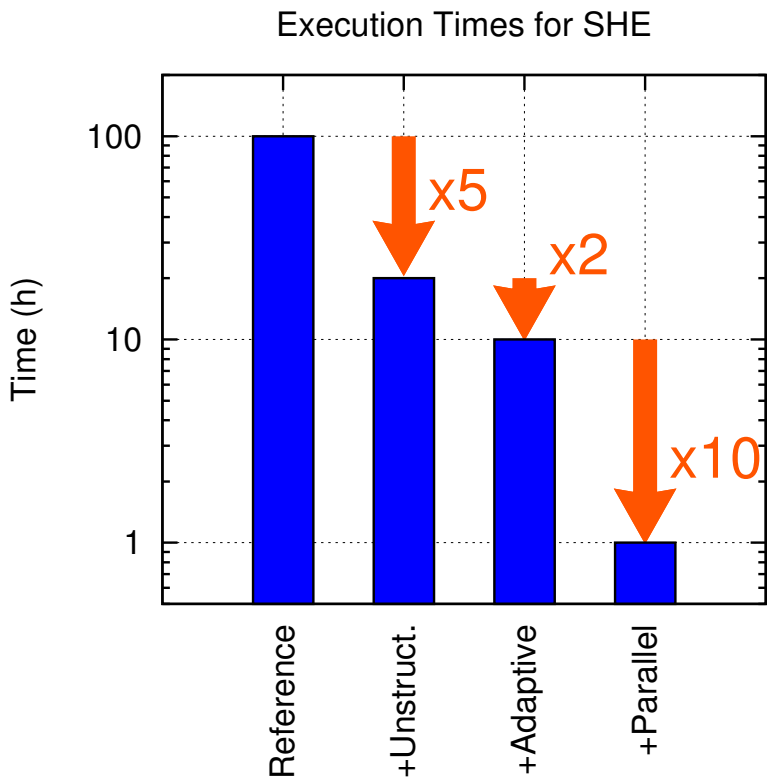
Electron Concentration (cm^{-3})

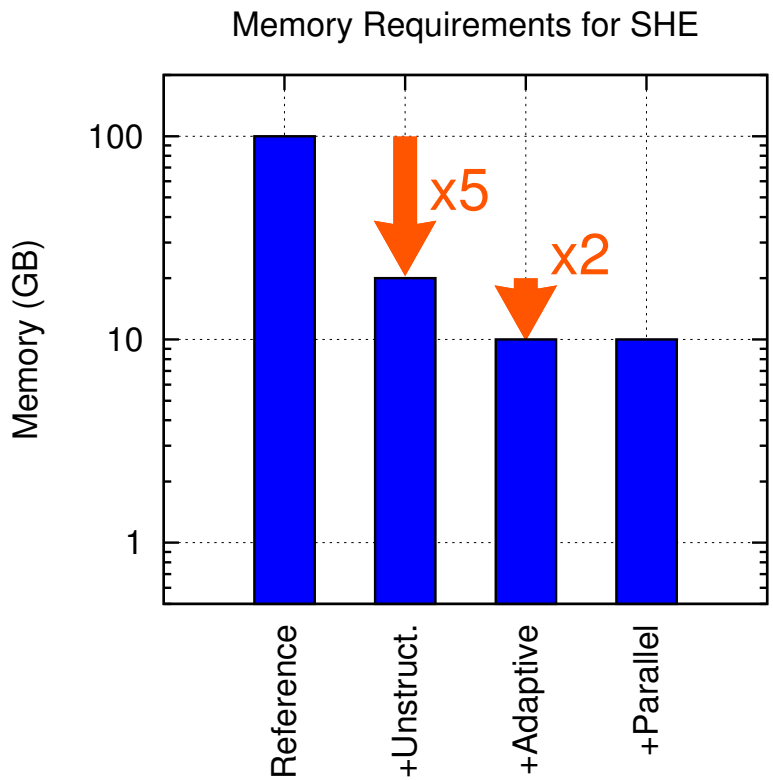


Electron Density with Energy above 1eV (cm^{-3})



Summary


Execution Times for SHE
Time (h)
100
10
1
x5
x2
x10
Reference
+Unstruct.
+Adaptive
+Parallel


Memory Requirements for SHE
Memory (GB)
100
10
1
x5
x2
Reference
+Unstruct.
+Adaptive
+Parallel

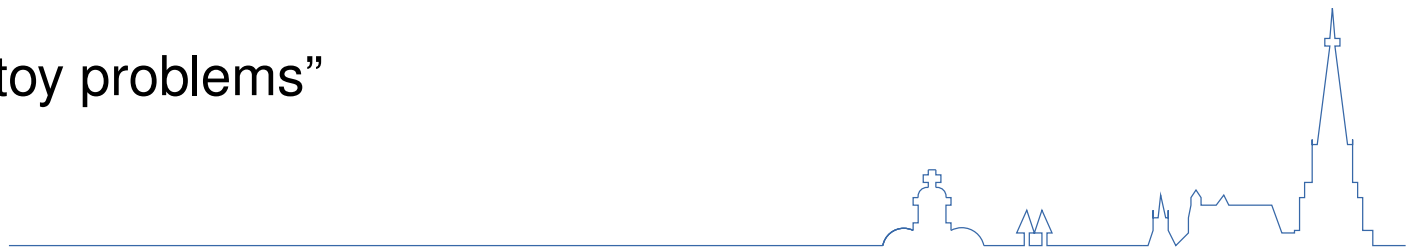
ViennaSHE

Features

- Unstructured grids in 1d, 2d, 3d
- Adaptive variable-order expansions
- Parallelization (shared memory, GPUs)
- Carrier-carrier scattering
- Free open source MIT/X11 license

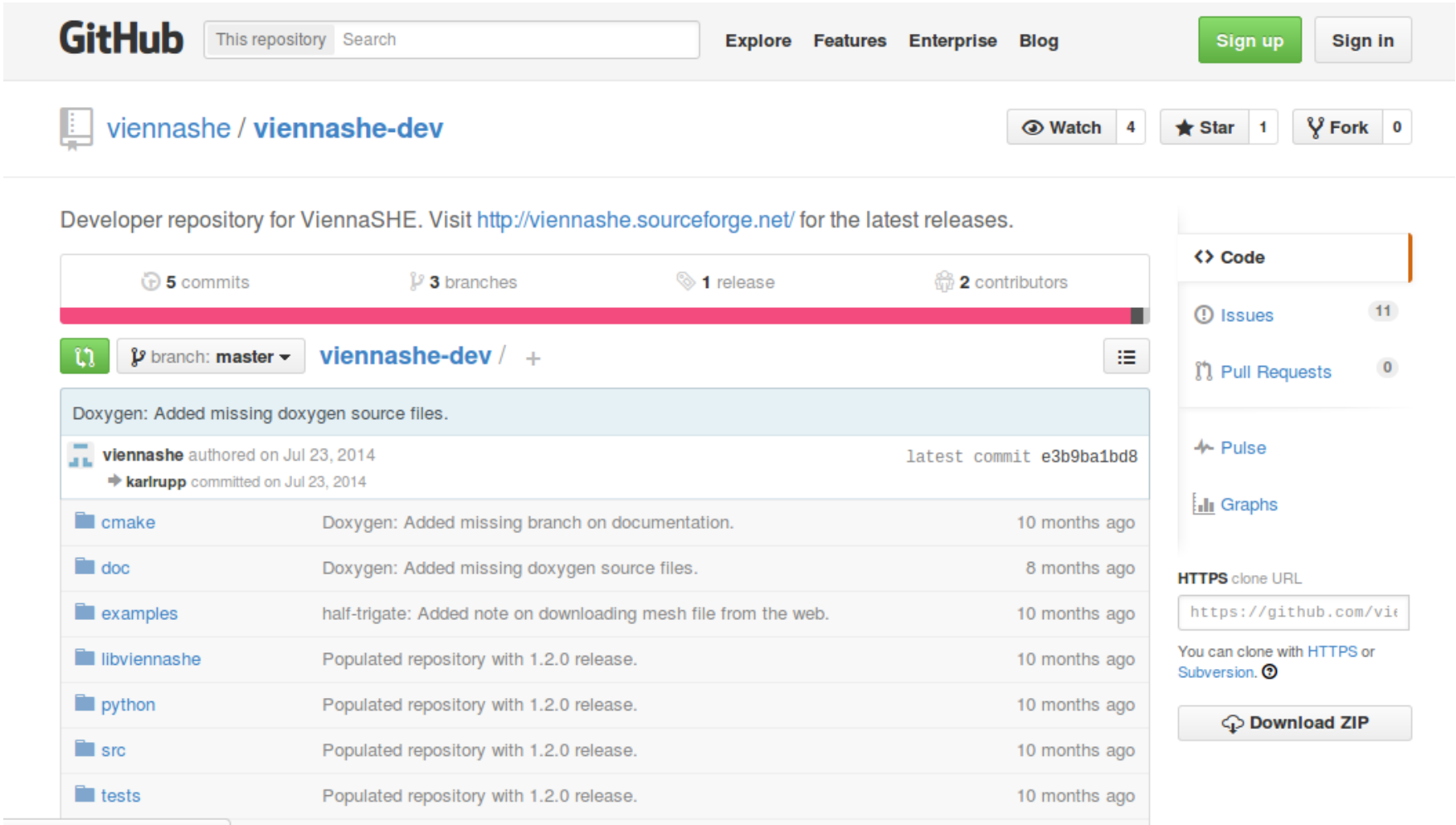
Rationale

- Open Science
- Reproducibility
- Extensibility
- “More than toy problems”



Development Infrastructure

Developer Repository on GitHub



Development Infrastructure

Nightly Test Suite

Nightly

Site	Build Name	Update	Configure		Build		Test			Build Time
		Files	Error	Warn	Error	Warn	Not Run	Fail	Pass	
jwein3	Darwin-GCC-4.2.1-Debug-master		0	0	0	0	0	1	28	Mar 12, 2015 - 08:45 UTC
jwein3	Darwin-GCC-4.2.1-Debug-next		0	0	0	0	0	1	29	23 hours ago
centos5	Linux-GCC-4.1.2-Debug-master		0	0	0	0	0	1	28	21 hours ago
centos5	Linux-GCC-4.1.2-Debug-next		0	0	0	0	0	1	29	22 hours ago
jwein3	Darwin-GCC-4.2.1-Release-master		0	0	0	0	0	0	29	23 hours ago
jwein3	Darwin-GCC-4.2.1-Release-next		0	0	0	0	0	0	30	23 hours ago
krupp2	Linux-Clang-3.3-Debug-master		0	0	0	0	0	0	29	Mar 12, 2015 - 04:34 UTC
krupp2	Linux-Clang-3.3-Debug-next		0	0	0	0	0	0	30	Mar 12, 2015 - 03:58 UTC
krupp2	Linux-Clang-3.3-Release-master		0	0	0	0	0	0	29	Mar 12, 2015 - 04:05 UTC
krupp2	Linux-Clang-3.3-Release-next		0	0	0	0	0	0	30	Mar 12, 2015 - 03:28 UTC
centos5	Linux-GCC-4.1.2-Release-master		0	0	0	0	0	0	29	21 hours ago
centos5	Linux-GCC-4.1.2-Release-next		0	0	0	0	0	0	30	23 hours ago
centos5	Linux-GCC-4.4.7-Debug-master		0	0	0	0	0	0	29	22 hours ago
centos5	Linux-GCC-4.4.7-Debug-next		0	0	0	0	0	0	30	23 hours ago
centos5	Linux-GCC-4.4.7-Release-master		0	0	0	0	0	0	29	22 hours ago
centos5	Linux-GCC-4.4.7-Release-next		0	0	0	0	0	0	30	23 hours ago
krupp2	Linux-GCC-4.8.2-Debug-master		0	0	0	0	0	0	29	Mar 12, 2015 - 04:07 UTC
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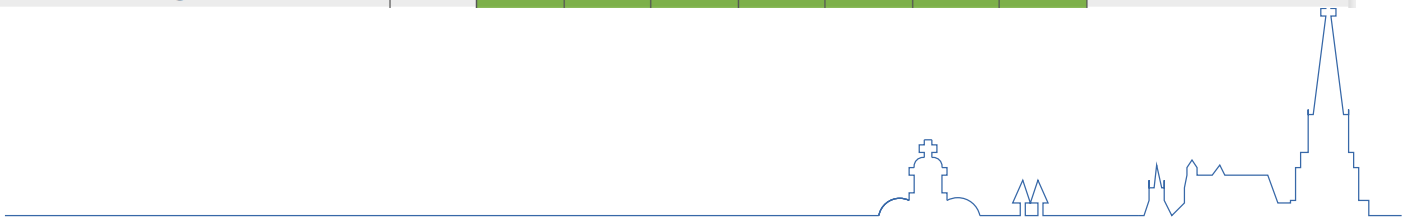

Development Infrastructure

Library Centric Development

Applications: ViennaCLBench ViennaMOS ViennaProfiler ViennaSHE ViennaWD ViennaX
Libraries: ViennaCL ViennaData ViennaFEM ViennaGrid ViennaIPD ViennaMath ViennaMesh

ViennaSHE

Content

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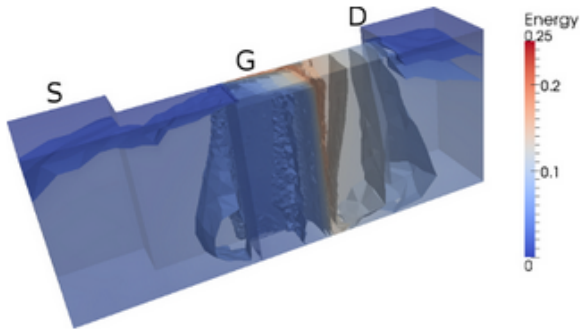
May 9th, 2014: ViennaSHE 1.2.0 released! (Changelog)

ViennaSHE is a free, multi-dimensional semiconductor device simulator using Spherical Harmonics Expansions for deterministic numerical solution of the Boltzmann Transport Equation. The method provides much shorter execution times than Monte Carlo methods at comparable accuracy, thus making it an ideal candidate for next-generation TCAD. In addition to traditional macroscopic models such as drift-diffusion, which can also be solved using ViennaSHE, the full carrier distribution functions are computed. This provides full information about the carrier energy distribution, which is for example of utmost importance for the study of hot carrier degradation.



http://viennashe.sourceforge.net/

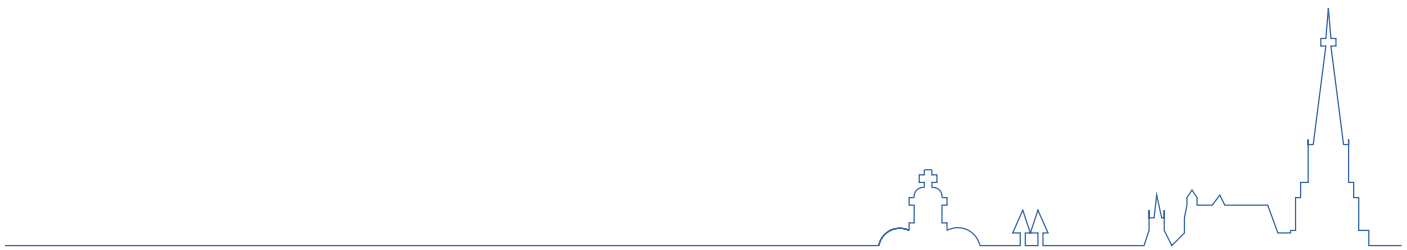
User Requirements

Input/Output

- Reader/writer for commercial file formats
- Material parameter tweaks
- Robustness of solver

Lessons Learnt

- C++ is a golden cage
- Long-term investments in research hard
- Each parameter needs to adjustable



Conclusion

SHE Method

- Viable alternative to Monte Carlo
- Full 3d device simulations possible
- Convergence behavior similar to drift-diffusion model

ViennaSHE

- Free open source simulator based on SHE method
- Fully open development infrastructure
- http://viennashe.sourceforge.net/

Thanks to the organizers for AMaSiS 2015!