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Miniapplications: a Promising Approach to Improve the Performance of Computational Mechanics Codes

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Motivation and Goals

- Engineering application codes (“app”) are huge and complex
- Typically Herculean effort to change algorithms
  - Difficult to evaluate new algorithms
  - Difficult to evaluate different programming paradigms
  - Impractical for “co-design” of architecture, programming languages and algorithms
    - E.g.: app took 4-6 months to port (twice)
    - US national lab codes export controlled
- Miniapplications (“miniapps”)
  - Proxy for key app performance issue
  - Easy to port, open source
  - Mantevo

Motivation and Goals

- But is miniapp representative of app?
  - Intuitively one would think so… (more like hope)
  - Improperly designed miniapp or use of a miniapp outside its scope will produce useless results, or worse, misleading results
- Talk will focus on comparison of an FEM semiconductor device modeling app and an FEM miniapp
- Key questions:
  - What is miniapp not intended to represent?
  - What is miniapp intended to represent?
  - How good of a job does it do?

Application Proxies

- Proxy App: Generic term for all types
- Skeleton App:
  - Communication accurate, computation fake
- Compact App:
  - Small version of app; attempt some tie to physics
- Scalable Synthetic Compact Applications (SSCA):
  - DARPA HPCS
- HPC Challenge Benchmarks
- NAS Parallel Benchmarks
- SPEC
- Others (e.g. Seven Dwarfs, etc.)

Miniapps Specifications

- Size: O(1K) lines
- Focus: Proxy for key app performance issue
- Availability: Open Source
- Scope of allowed change: Any and all
- Intent
  - Improving performance of app
  - Co-design: architecture and app
- Reference version developer & owner: *Application team*

Mantevo Project

(Heroux et al.)

- Multi-faceted application performance project
- Started 5 years ago
- Two types of packages:
  - Miniapps: Small, self-contained programs
    - MiniFE/HPCCG: unstructured implicit FEM/FVM
    - phdMesh: explicit FEM, contact detection
    - MiniMD: MD Force computations
    - MiniXyce: Circuit RC ladder
    - MiniGhost: Data exchange pattern of CTH
    - And many more coming online…
  - Minidrivers: Wrappers around Trilinos packages.
    - Beam: Intrepid+FEI+Trilinos solvers
    - Epetra Benchmark Tests: Core Epetra kernels
- Open Source (LGPL)

Are Miniapps Representative of Apps? Focus on an FEM App and Miniapp

- Work in progress, building a “body of evidence,” the more data, the better
- Comparison of semiconductor device modeling app to miniapp
- Single compute node comparison
  - Effects of memory bandwidth
  - Cache performance
- Future directions: Comparison at scale

RAMSES/Charon Semiconductor Device Simulator

Charon team: G. Hennigan (PI), R. Hoekstra, J. Castro, D. Fixel, R. Pawlowski, E. Phipps, L. Musson, T. Smith, J. Shadid, Lin

- Drift-diffusion model for semiconductor devices
- Stabilized FEM and FVM discretization for unstructured meshes
- Fully-implicit Newton-Krylov solver; usually GMRES
  - Robust, but need efficient solution of sparse linear systems
- Massively parallel for high fidelity simulations
- Trilinos for nonlinear solver (NOX), Krylov solver (AztecOO), preconditioner (ML and Ifpack), Sacado for AD (matrix assembly)

Semiconductor Drift-Diffusion Model

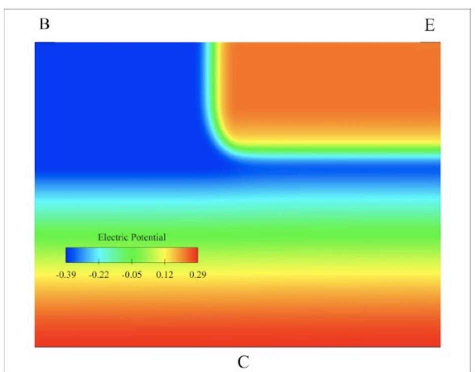
Electric potential $$-\nabla \cdot \epsilon \nabla \psi = q\,(p - n + C)$$

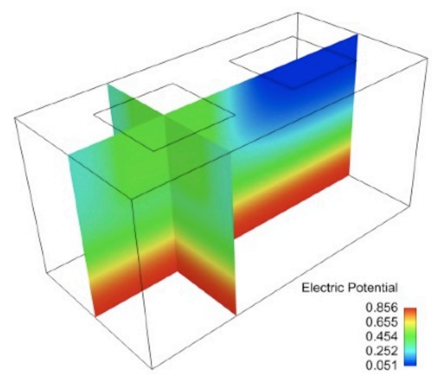
$$\nabla \cdot \mathbf{J}_n - qR = q\frac{\partial n}{\partial t} \qquad \mathbf{J}_n = -qn\mu_n \nabla \psi + qD_n \nabla n$$

$$-\nabla \cdot \mathbf{J}_p - qR = q\frac{\partial p}{\partial t} \qquad \mathbf{J}_p = -qp\mu_p \nabla \psi - qD_p \nabla p$$

- ψ: electric potential
- n: electron concentration
- p: hole concentration
- C: doping profile
- R: generation-recombination term

Defect species: each additional species adds a transport-reaction equation





2D and 3D steady-state drift-diffusion bipolar junction transistor (BJT) test cases (G. Hennigan)

Implicit Finite Element Miniapp: MiniFE

(A. Williams)

- Steady-state 3D heat equation (Poisson equation)
- Geometry is a cube
- Finite element method with hexahedral elements
- FEM Matrix and RHS assembly
- Symmetric matrix solved by CG (no preconditioner)

- What is MiniFE not intended to represent?
  - App with different physics: Number of Newton steps, number of Krylov iterations per Newton step
- What is MiniFE intended to represent?
  - Krylov solve (dominant computational kernel)
  - Matrix and RHS assembly (but may not hold if app uses different approach)

MiniFE Represent App? Memory Bandwidth Effects

- Dual-Socket 12-core Magny-Cours; 31k DOF/core; Intel 11
- Charon steady-state drift-diffusion BJT
- 2D App (3 DOF/node) vs. 3D MiniFE; match DOF/core and NNZ
- Efficiency: ratio of 4-core time to n-core time (expressed as %)
- LS and PS+LS: linear solve without/with ML precond setup time

MiniFE

cores	CG eff
4	Ref
8	87
12	74
16	64
20	56
24	46

Charon

cores	LS eff	PS+LS eff
4	Ref	Ref
8	88	89
12	77	80
16	68	72
20	59	64
24	52	57

MiniFE Represent App? MC: Cache Performance

- Cray XE6 node (dual-socket 2.4GHz 8-core Magny-Cours); 16 MPI processes (use all 16 cores); 31k DOF/core
- 2D Charon steady-state drift-diffusion BJT
- GCC 4.5.2 compiler; PAPI 4.1.2
- 2D App (3 DOF/node) vs. 3D MiniFE; match DOF/core and NNZ
- Compare matrix and RHS assembly time

MiniFE

	CG	Mat+RHS
L1 HR	99.8	99.9
L2 HR	95	67
L3 HR	13	48

Charon

	LS	PS+LS	Mat+RHS
L1 HR	99.2	99.7	99.7
L2 HR	81	80	98.3
L3 HR	17	22	98.4

Abbreviations: HR (hit rate), LS (linear solve), PS (prec setup)

MiniFE Represent App? Nehalem: Cache Performance

- Dual-socket 2.93 GHz quadcore Nehalem; 8 MPI ranks; 31k DOF/core
- 2D Charon steady-state drift-diffusion BJT
- Intel 11; OpenMPI 1.4.3; PAPI 4.1.3
- 2D Charon (3 DOF/node) vs. 3D MiniFE; match DOF/core and NNZ
- Compare matrix and RHS assembly time

MiniFE

	CG	Mat+RHS
L1 HR	88	99.9
L2 HR	3	29
L3 HR	15	15

Charon

	LS	PS+LS	Mat+RHS
L1 HR	91	91	97
L2 HR	7	7	88
L3 HR	19	19	94

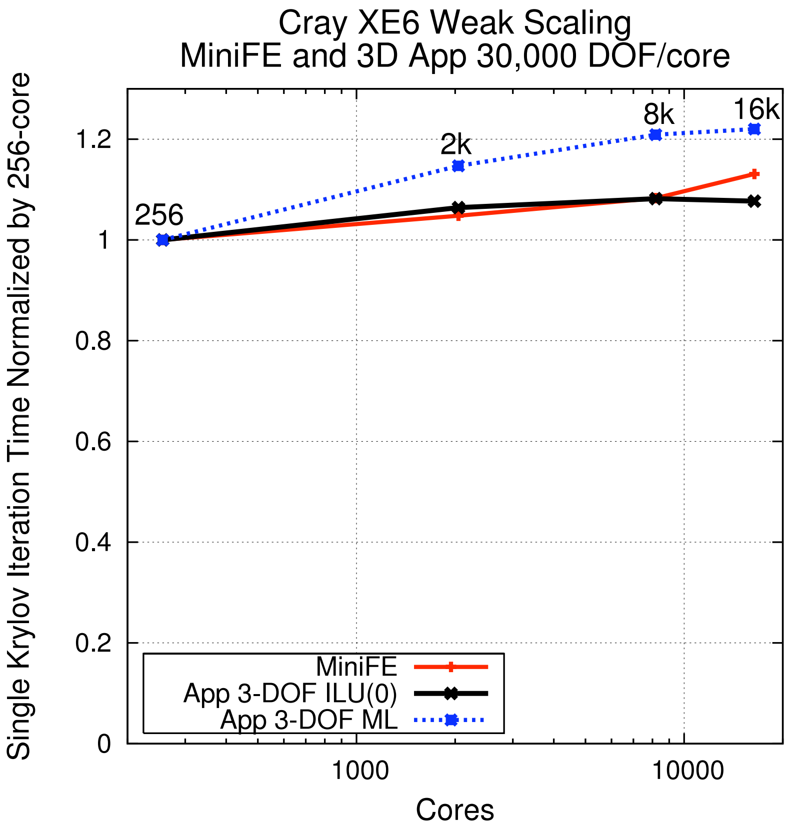
Abbreviations: HR (hit rate), LS (linear solve), PS (prec setup)

MiniFE Represent 3D App? Cache Performance

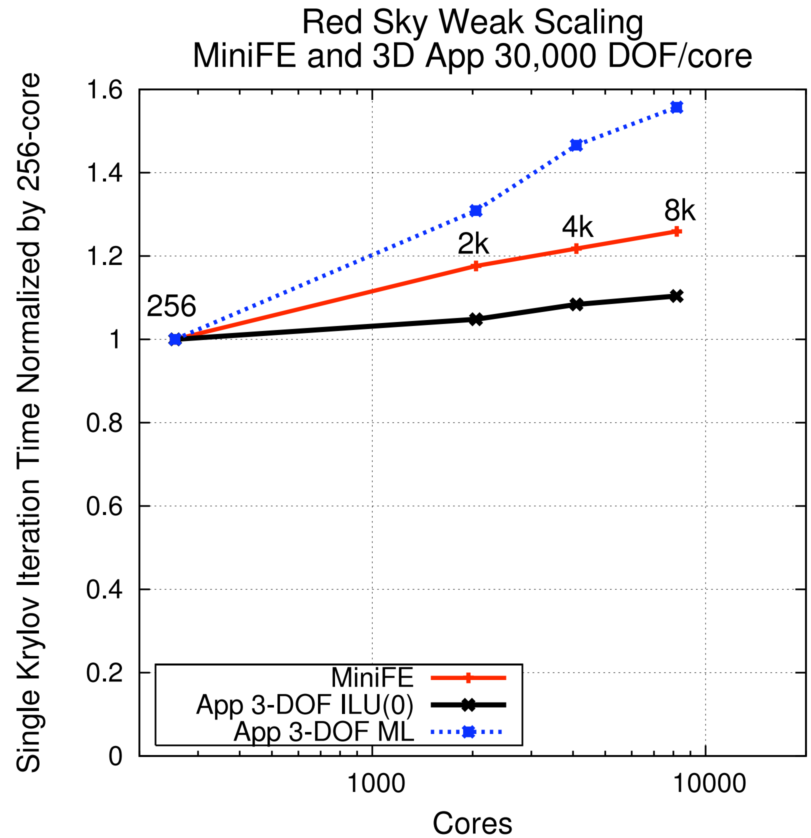
- 3D Charon steady-state BJT
- Cray XE6; dual-socket 2.4GHz 8-core Magny-Cours; 16 MPI ranks
- App Aztec Krylov solver
  - 1 DOF/node with BiCGSTAB; ILU(0)ov=0 precond (“ILU/bicg”)
  - 3 DOF/node with BiCGSTAB; ILU(0)ov=0 precond (“ILU/bicg”)
  - 3 DOF/node with GMRES; ILU(0)ov=0 precond (“ILU/GMR”)
  - 3 DOF/node with GMRES; ML multigrid precond

	MiniFE	3D Charon (Aztec)			
	1 DOF/node	1 DOF/node	3 DOF/node		
	CG	ILU/bicg	ILU/bicg	ILU/GMR	ML/GMR
L1 HR	99.8	99.2	99.3	99.5	99.5
L2 HR	95	84	82	91	89
L3 HR	13	14	7	19	15

Future Directions: Comparison at Scale



Cray XE6



Red Sky (Nehalem linux cluster)

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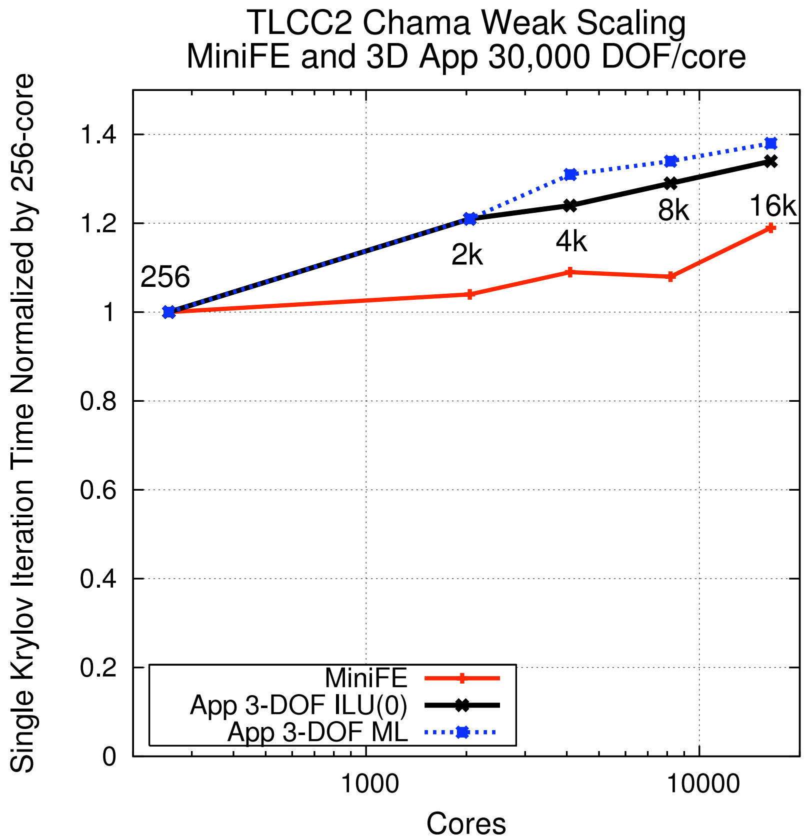
Future Directions: Comparison at Scale



Sandy Bridge linux cluster (fat tree)

Conclusions and Future Work

- Difficult to work with large apps: miniapps can help
  - Evaluating new algorithms to improve performance
  - Co-design
- Need to understand what the miniapp is intended to represent as well as what it is not intended to represent
- Performing a study to understand how well MiniFE can represent an FEM app
  - Seems to be a reasonable performance proxy for single compute node
  - Doesn't do as well at scale; further investigation is needed to understand discrepancies
- Future work
  - More rigorous framework for comparisons
  - Make miniFE more predictive of MG preconditioner
  - Use miniapp to improve app

Thanks For Your Attention!

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Extra Slides

MiniFE Represent App? Processor/Node Ranking

- Charon steady-state drift-diffusion BJT; 8 MPI tasks; 31k DOF/core
- Nehalem (Intel 11; all cores of dual-socket quadcore)
- 12-core Magny-Cours (Intel 11; one socket, 4 MPI tasks/die)
- Barcelona (Intel 11; two sockets out of the quad-socket)
- 2D App (3 DOF/node) vs. 3D MiniFE; match DOF/core and NNZ
- LS and PS+LS: linear solve without/with ML precond setup time
- Compare matrix and RHS assembly time

MiniFE

	CG	Mat+RHS
1	Nehalem	Nehalem
2	MC(1.7)	MC(1.7)
3	Barc(2.7)	Barc(1.8)

Charon

	LS	PS+LS	Mat+RHS
1	Nehalem	Nehalem	Nehalem
2	MC(1.7)	MC(1.8)	MC(1.46)
3	Barc(2.8)	Barc(2.5)	Barc(1.52)

Number in parenthesis is factor greater than #1 time

MiniFE Represent App? Compiler Ranking

- Quad-socket quadcore Barcelona node; 16 tasks; 31k DOF/core
- Charon steady-state drift-diffusion BJT
- Intel 11.1.064; PGI 9.0.4; GNU 4.3.4 (all Open MPI 1.4.1)
- 2D App (3 DOF/node) vs. 3D MiniFE; match DOF/core and NNZ
- LS and PS+LS: linear solve without/with ML precond setup time
- Compare matrix and RHS assembly time

MiniFE

	CG	Mat+RHS
1	Intel	Intel
2	GNU(1.01)	GNU (1.1)
3	PGI(1.04)	PGI (1.8)

Charon

	LS	PS+LS	Mat+RHS
1	Intel	Intel	Intel
2	GNU(1.02)	GNU(1.01)	GNU(2.5)
3	PGI(1.06)	PGI(1.2)	PGI(3.3)

Number in parenthesis is factor greater than #1 time