How to Choose an Algorithm

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RELACS People





How do we choose an algorithm?

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We choose the fastest one...

Timing is tricky. It's sensitive to

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machine characteristics

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problem details

Computation (HPL)

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Bandwidth (Roofline)

Computation (HPL)

Bandwidth (Roofline)

Latency (LogP)

Computation (HPL) Bandwidth (Roofline) Latency (LogP) Concurrency

Does this implementation scale weakly?

Does this implementation scale weakly? strongly?

Is one implementation more efficient than another on this machine?

What about questions like...

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Should I discretize this

problem with CG or DG?

What about questions like...

Should I solve using the

Picard or Newton Method?

The key notion we are missing is

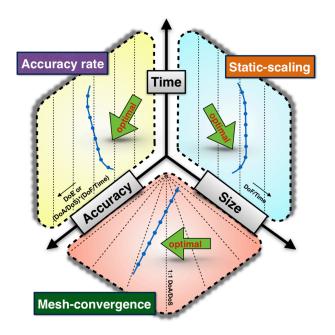
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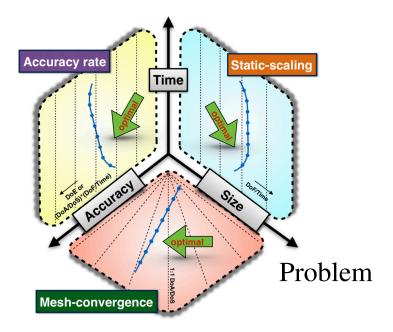
accuracy

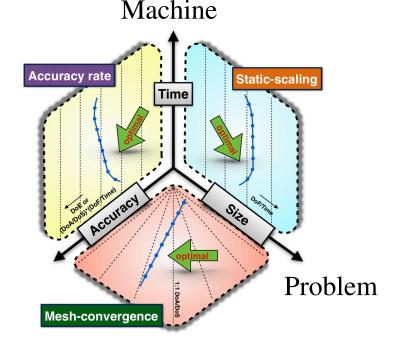
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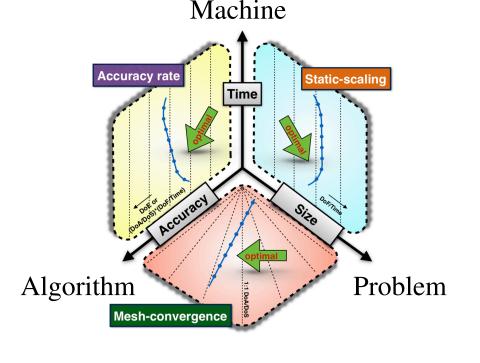
accuracy

It distinguishes algorithms with different convergence behavior (Chang et al. 2018)

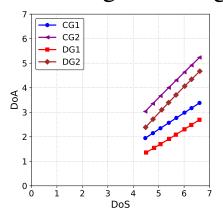




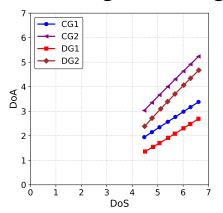




Mesh Convergence Diagram

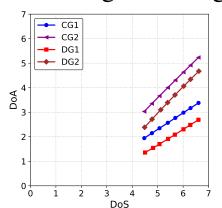


Mesh Convergence Diagram

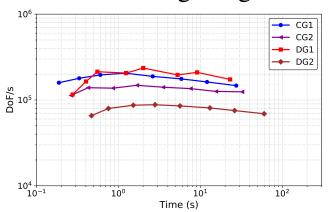


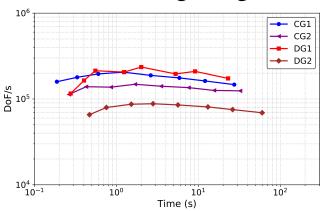
1/error vs. size

Mesh Convergence Diagram

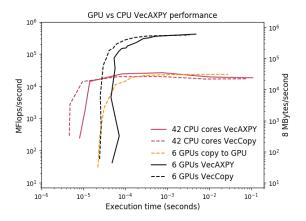


Does my Algorithm solve this Problem?

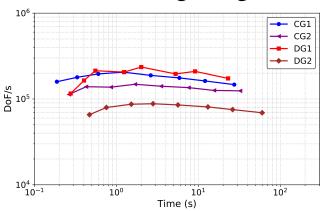




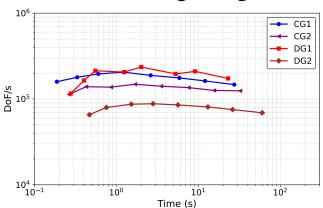
size/time vs. time



size/time vs. time



size/time vs. time



Is my Algorithm efficient on this Machine?

How should we measure accuracy?

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accuracy rate $\frac{e}{T}$

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Marginal accuracy rate falls off steeply with problem size

Consider an optimal PDE solver:

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$$T = Wh^{-d}$$
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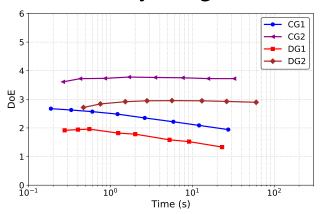
$$T = Wh^{-d}$$
 and $e = Ch^{\alpha}$

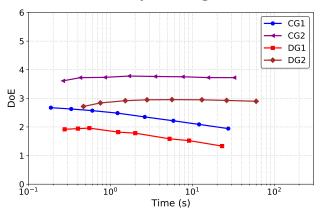
The error-time has a simple form

$$-\log(e \cdot T)$$

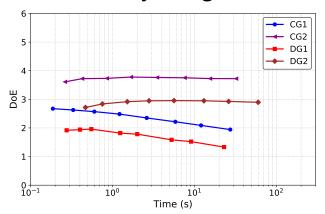
$$= -\log(Ch^{\alpha}Wh^{-d})$$

$$= (d - \alpha)\log(h) - \log(CW)$$

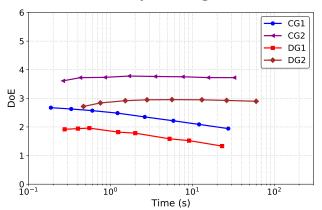




1/error-time vs. time



$$\frac{1/\text{error}}{\text{size}} \times \frac{\text{size/time}}{\text{time}} = \frac{1/(\text{error} \cdot \text{time})}{\text{time}}$$



Does my Algorithm solve this Problem efficiently on this Machine?

Efficacy vs. Static Scaling

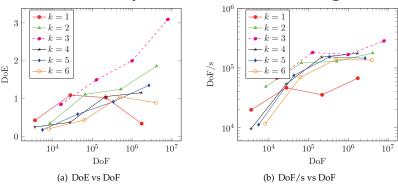


Figure 17: Time-accuracy performance analysis for the nearly incompressible problem ($\lambda = 10^6$).

(Fabien 2019)

Communication-Avoiding (CA) algorithms have exciting lower bounds

(Ballard et al. 2011)

CA TSQR is a great success (Demmel et al. 2012)

CA Krylov not a success

CA Krylov not a success

Accuracy depends on coarse grid communication in preconditioner

Future Questions:

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Is there a variational characterization of optimal algorithms?

Future Questions:

Can we think of error-time as an Algorithmic Action?

References I

- Chang, Justin, Maurice S. Fabien, Matthew G. Knepley, and Richard T. Mills (2018). "Comparative study of finite element methods using the Time-Accuracy-Size (TAS) spectrum analysis". In: SIAM Journal on Scientific Computing 40.6, pp. C779–C802. DOI: 10.1137/18M1172260. eprint: 1802.07832.
- Fabien, Maurice S. (2019). "A GPU-Accelerated Hybridizable
 Discontinuous Galerkin Method for Linear Elasticity". In:

 Communications in Computational Physics 27.2, pp. 513–545. ISSN:
 1991-7120. DOI: 10.4208/cicp.OA-2018-0235.
- Ballard, Grey, James Demmel, Olga Holtz, and Oded Schwartz (2011). "Minimizing Communication in Numerical Linear Algebra". In: SIAM Journal on Matrix Analysis and Applications 32.3, pp. 866–901. DOI: 10.1137/090769156.
- Demmel, James, Laura Grigori, Mark Hoemmen, and Julien Langou (2012). "Communication-optimal Parallel and Sequential QR and LU Factorizations". In: SIAM Journal on Scientific Computing 34.1, A206–A239. DOI: 10.1137/080731992.