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ADAPTATIONS OF PDE-BASED CODES TO EXTREME SCALE

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ABSTRACT

Adaptations to use next-generation computers closer to their potential are underway throughout scientific computing, including the important domains of CFD and other PDE-based models. Instead of squeezing out flops – the traditional goal of algorithmic optimality, which once served as a reasonable proxy for all associated costs (whether counting execution time or energy consumed) – algorithms must now put the squeeze on synchronizations, memory, and data transfers, while extra flops on locally cacheable data typically represent only small costs in time and energy. The scalable solvers employed in today's PDE-based codes, in particular, exploit frequent global synchronizations. After decades of programming model stability with bulk synchronous processing (BSP) based on domain decomposition implemented in the message passing interface (MPI), new programming models must be co-designed with the hardware. This architecture-induced evolution coincides with an evolution in capabilities demanded of the models, such as optimization, data assimilation, parameter identification (inverse problems), and uncertainty quantification. This talk will briefly recap the architectural constraints and outline future directions. We will illustrate with KAUST implementations of scalable solvers for emerging many core and GPU architectures.

REFERENCES

Background papers

CAI, X.-C., GROPP, W. D., KEYES, D. E. & TIDRIRI, M. D. (1994), Newton-Krylov-Schwarz Methods in CFD, in *Proceedings of the International Workshop on Numerical Methods for the Navier-Stokes Equations*, (F. Hebeker & R. Rannacher, eds.), Notes in *Numerical Fluid Mechanic*s, Vieweg Verlag, Braunschweig, pp. 17–30.

KNOLL, D. A. & KEYES, D. E. (2004), Jacobian-Free Newton-Krylov Methods: A Survey of Approaches and Applications, *J. Computational Physics*, **193**:357–397.

CAI, X.-C. & KEYES D. E. (2002), Nonlinear Preconditioned Inexact Newton Algorithms, *SIAM J. Scientific Computing*, **24**:183–200.

Gordon Bell Prize paper

GROPP, W. D., KAUSHIK, D. K., KEYES D. E. & SMITH, B. F. (2001), High Performance Parallel Implicit CFD, *Parallel Computing*, **27**:337–362.

Recent personal and community papers on high-end computational physics

KEYES, D. E. (2011), Exaflop/s – the Why and the How, *Comptes Rendus* **339**:70–77.

DONGARRA, J., P. BECKMAN, T. MOORE, P. AERTS, G. ALOISIO, J.-C. ANDRE, D. BARKAI, J.-Y. BERTHOU, T. BOKU, B. BRAUNSCHWEIG, F. CAPPELLO, B. CHAPMAN, X. CHI, A. CHOUDHARY, S. DOSANJH, T. DUNNING, S. FIORE, A. GEIST, W. D. GROPP, R. HARRISON, M. HERELD, M. HEROUX, A. HOISIE, K. HOTTA, Y. ISHIKAWA, Z. JIN, F. JOHNSON, S. KALE, R. KENWAY, D. KEYES, W. KRAMER, J. LABARTA, A. LICHNEWSKY, T. LIPPERT, R. LUCAS, B. MACCABE, S. MATSUOKA, P. MESSINA, P. MICHIELSE, B. MOHR, M. MUELLER, W. NAGEL, H. NAKASHIMA, M. E. PAPKA, D. REED, M. SATO, E. SEIDEL, J. SHALF, D. SKINNER, M. SNIR, T. STERLING, R. STEVENS, F. STREITZ, R. SUGAR, S. SUMIMOTO, W. TANG, J. TAYLOR, R. THAKUR, A. TREFETHEN, M. VALERO, A. VAN DER STEEN, J. VETTER, P. WILLIAMS, R. WISNIEWSKI & K. YELICK (2011), The International Exascale Software Roadmap, *Int. J. High Performance Computing Applications*, **25**:1–82.

KEYES, D. E., L. C MCINNES, C. WOODWARD, W. GROPP, E. MYRA, C. FARHAT, M. PERNICE, J. BELL, J. BROWN, A. CLO, J. CONNORS, E. CONSTANTINESCU, D. ESTEP, K. EVANS, C. FARHAT, A. HAKIM, G. HAMMOND, G. HANSEN, J. HILL, T. ISAAC, X. JIAO, K. JORDAN, D. KAUSHIK, E. KAXIRAS, A. KONIGES, K. LEE, A. LOTT, Q. LU, J. MAGERLEIN, R. MAXWELL, M. MCCOURT, M. MEHL, R. PAWLOWSKI, A. P. RANDLES, D. REYNOLDS, B. RIVIERE, U. RUEDE, T. SCHEIBE, J. SHADID, B. SHEEHAN, M. SHEPHARD, A. SIEGEL, B. SMITH, X. TANG, C. WILSON & B. WOHLMUTH (2013), Multiphysics Simulations: Challenges and Opportunities, *Int. J. High Performance Computing Applications*, **27**:5–83.

Recent technical papers on algorithms and implementations for emerging architectures

LIU, L. & KEYES, D. E. (2015), Field-split preconditioned inexact Newton algorithms, *SIAM Journal on Scientific Computing*, **37**:A1388–A1409.

ALFARHAN, M., KAUSHIK, D., & KEYES, D. E. (2015), Unstructured computational aerodynamics on many integrated core architecture, *Parallel Computing (under review).*

