# Mathematical computations related abstracts for 2018 BOUT++ Workshop

Prepared by LLNL for USDOE SC-FES under Contract DE-AC52- 07NA27344. LLNL-ABS-755708.

# Using VisIt to Visualize BOUT++ data

Eric Brugger, LLNL

VisIt is a general purpose, open source visualization and data analysis tool that runs on a variety of platforms including Linux, Mac OSX and Windows. It contains functionality for data exploration, quantitative analysis, making presentation graphics, visual debugging, and comparative analysis. VisIt supports a graphical user interface as well as a powerful Python scripting interface. VisIt includes a database reader that reads NetCDF based BOUT++ files. During this presentation I will provide a brief overview of using VisIt followed by information specific to visualizing BOUT++ data. I will also discuss recent changes to the interpolation scheme for mapping BOUT++ data onto a 3D grid that improves the performance and quality of the 3D imagery. Furthermore, I will present several Python scripts that make it easy for users to create standard images and animations from BOUT++ data, replacing minutes of user interaction with the execution of a macro.

# A scalable, fully implicit algorithm for the low-$\beta$ extended MHD model

L. Chacón and A. Stanier
Los Alamos National Laboratory
Los Alamos, NM 87545

The low-$\beta$ extended magnetohydrodynamics (low-$\beta$ XMHD) model is obtained by taking the large-guide-field and cold-ion limit of the extended MHD model. The resulting model is appealing owing to its simplicity (it is a small set of scalar equations), and because it describes a wide range of laboratory magnetic confinement devices, the solar corona, and other astrophysical plasmas in which large guide fields are present. However, the numerical integration of the low-$\beta$ XMHD system is non-trivial due to the presence of disparate time and length scales, which demand both spatial adaptivity and efficient implicit integration methods for efficiency. The large time-scale disparity originates in the presence of fast dispersive waves, which result in significant numerical stiffness and the need of high-order dissipation operators to prevent numerical noise in nonlinear regimes. Both dispersive hyperbolic systems and high-order differential operators stress numerical algorithms, and benefit from an implicit treatment.

Despite the relevance of the low-$\beta$ XMHD system in the study of magnetized plasmas, to our knowledge there is scant effort devoted towards the development of modern, efficient implicit algorithms for the numerical solution of the low-$\beta$ XMHD model. There are several efforts in the literature record that employ implicit timestepping,[1,2,3] but only Ref. [3] makes an effort to characterize the solver performance. It employs a Newton-Krylov-Schwarz implicit parallel solver, with incomplete ILU methods with various degrees of overlap in each parallel domain. Performance is quite sensitive to the domain overlap, and iteration count is quite high, but scales reasonably well in parallel. Reported speedups with respect to explicit approaches are at most of an order of magnitude for a $1980\times1980$ mesh.

The focus of this paper is to demonstrate an efficient, optimal nonlinearly implicit algorithm for the low-$\beta$ XMHD model.[4] The approach uses Jacobian-free Newton-Krylov (JFNK) methods, effectively preconditioned using physics-based approximations of the Jacobian system that are multigrid-friendly, and therefore deliver optimal convergence rates. The preconditioning approach presented here leverages earlier developments of effective physics-based preconditioners for MHD[5] and extended MHD,[6] and in particular employs a similar parabolization strategy to that presented in these studies. We demonstrate the performance of the algorithm with challenging numerical examples. In particular, we demonstrate optimal algorithmic scaling under mesh refinement, and excellent weak parallel scaling up to 4096 cores. CPU speedups with respect to explicit methods beyond 3 orders of magnitude are demonstrated with the largest processor counts. We apply the algorithms to the problem of fast reconnection in the large-guide-field regime to derive new physical insights for this challenging problem.

---

[1] G. T. A. Huysmans, *Plasma Phys. Control. Fusion,* **47** (2005)

[2] K. Germaschewski, A. Bhattacharjee, and C.-S. Ng, "The magnetic reconnection code: an AMR-based fully implicit simulation suite," in Numerical Modeling of Space Plasma Flows (N. B. Pogorelov and G. P. Zank, eds.), vol. 359 of ASP Conference Series, 2006.

[3] S. Ovtchinnikov, F. Dobrian, X.-C. Cai, and D. Keyes, *J. Comput. Phys.*, **225** (2007).

[4] L. Chacón and A. Stanier, *J. Comput. Phys.*, **326** (2016)

[5] L. Chacón, D. A. Knoll, and J. M. Finn, *J. Comput. Phys.*, **178** (2002)

[6] L. Chacón and D. A. Knoll, *J. Comput. Phys.*, **188** (2003)

## The SUNDIALS Suite of Time Integrators and Nonlinear Solvers

David James Gardner
Lawrence Livermore National laboratory

SUNDIALS is a suite of robust and scalable solvers for systems of ordinary differential equations, differential-algebraic equations, and nonlinear equations. The suite consists of six packages: CVODE(S), ARKode, IDA(S), and KINSOL. Each package is built on a common vector and linear solver API allowing for application-specific and user-defined linear solvers and data structures, encapsulated parallelism, and algorithmic flexibility. As part of the DOE's Exascale Computing Program and FASTMath Institute, SUNDIALS is enabling time integrators for exascale architectures. In this presentation we will summarize capabilities of the SUNDIALS suite, overview current development efforts, and discuss incorporation of new work in multirate and parallel-in-time integration methods.

# High Performance Computing Resources at NERSC

Brian Ffriesen

Lawrence Berkeley National Laboratory

I present the high performance computing resources available at the National Energy Research Scientific Computing Center (NERSC) at Lawrence Berkeley National Laboratory. NERSC is the mission computing facility for the DOE Office of Science, supporting 7000 users in 49 states and 47 countries, contributing to 800 projects spanning all 6 programs in the Office of Science. I describe the architectural details of Cori and Edison, the two HPC systems currently in production at NERSC, as well as the software available to application developers who use those systems, including compilers, debuggers, and profiling tools. I briefly discuss future directions of computing at NERSC.

# Progress on Scalable Solution of Implicit FE Continuum Plasma Physics Models

John N. Shadid, Roger P. Pawlowski, Edward P. Phillips, Paul T. Lin, Sidafa Conde, SIbu Mabuza, Eric Cyr, Sean Miller

Sandia National Laboratory

The mathematical basis for the continuum modeling of plasma physics systems is the solution of the governing partial differential equations (PDEs) describing conservation of mass, momentum, and energy, along with various forms of approximations to Maxwell's equations. The resulting systems are characterized by strong nonlinear and nonsymmetric coupling of fluid and electromagnetic phenomena, as well as the significant range of time- and length-scales that these interactions produce. To enable accurate and stable approximation of these systems a range of spatial and temporal discretization methods are commonly employed. In the context of finite element spatial discretization methods these include mixed integration, stabilized and variational multiscale (VMS) methods, and structure-preserving (physics compatible) approaches. For effective long-time-scale integration of these systems the implicit representation of at least a subset of the operators is required.

Two well-structured approaches, of recent interest, are fully-implicit and implicit-explicit (IMEX) type time-integration methods employing Newton-Krylov type nonlinear/linear iterative solvers. To enable robust, scalable and efficient solution of the large-scale sparse linear systems generated by a Newton linearization, fully-coupled multilevel preconditioners are developed. The multilevel preconditioners are based on two differing approaches. The first technique employs a graph-based aggregation method applied to the nonzero block structure of the Jacobian matrix. The second approach utilizes approximate block factorization (ABF) methods and physics-based preconditioning approaches that reduce the coupled systems into a set of simplified sub-systems to which optimal multilevel methods are applied.

To demonstrate the flexibility of implicit/IMEX FE discretizations and the fully-coupled Newton-Krylov-AMG solution approaches various forms of resistive magnetohydrodynamic (MHD) and multifluid electromagnetic plasma models are considered. In this context, we first briefly discuss the mathematical models and formulations for a subset of these systems, and then present results for representative plasma physics problems of current interest. Additionally, the discussion considers the robustness, efficiency, and the parallel and algorithmic scaling of the preconditioning methods. Weak scaling results include studies on up to 1M cores.

*This work was supported by the DOE Office of Science Advanced Scientific Computing Research - Applied Math Research program and an ASCR/Office of Fusion Energy SciDAC Partnership Project at Sandia National Laboratories.

# Contemporary machine learning: techniques for practitioners in the physical sciences

Brian K. Spears
Lawrence Livermore National Laboratory

Machine learning is the science of using computers to find relationships in data without explicitly knowing or programming those relationships in advance. Often without realizing it, we employ machine learning every day as we use our phones or drive our cars. Over the last few years, machine learning has found increasingly broad application in the physical sciences. This most often involves building a model relationship between a dependent, measurable output and an associated set of controllable, but complicated, independent inputs. The methods are applicable both to experimental observations and to databases of simulated output from large, detailed numerical simulations.

In this tutorial, we will present an overview of current tools and techniques in machine learning – a jumping-off point for researchers interested in using machine learning to advance their work. We will discuss supervised learning techniques for modeling complicated functions, beginning with familiar regression schemes, then advancing to more sophisticated decision trees, modern neural networks, and deep learning methods. Next, we will cover unsupervised learning and techniques for reducing the dimensionality of input spaces and for clustering data. We'll show example applications from multiple scientific disciplines. Along the way, we will describe methods for practitioners to help ensure that their models generalize from their training data to as-yet-unseen test data. We will finally point out some limitations to modern machine learning and speculate on some ways that practitioners from the physical sciences may be particularly suited to help.

# Overview of the modular finite element methods

Tzanio Kolev
Lawrence Livermore National Laboratory

In this talk, we present an overview of the modular finite element methods (MFEM) library (mfem.org), including its main abstraction classes, their corresponding linear algebra objects, and implementation variants. We discuss the components required for the construction and application of general finite element discretization operators and the various choices for their software implementation, e.g. as a single assembled parallel CSR matrix, or as a product of linear operators, i.e. "matrix-free" representations. We highlight the pros and cons of the various choices based on the discretization parameters such as solution space order, mesh order, choice of quadrature, etc., and present numerical illustration with MFEM examples. We also report on the progress of the ongoing efforts to implement efficiently and integrate seamlessly support for architectures with accelerators (e.g. GPUs) in the library.

**Overview of Forward and Inverse Uncertainty Quantification Methods**

Tim Wildey[1]

[1]*Sandia National Labs: Optimization and UQ, Albuquerque, NM, USA*
*tmwilde@sandia.gov*

Uncertainty and error are ubiquitous in predictive modeling and simulation due to unknown model parameters and various sources of deterministic and stochastic error. Consequently, there is considerable interest in developing efficient and accurate methods to perform both forward uncertainty quantification (UQ): given uncertain model inputs, quantify the uncertainty in the outputs; and inverse UQ: given uncertain output data, quantify the uncertainty in the model inputs. The goal of this presentation is to give a high-level perspective on the various methods available to enable forward and inverse propagation of uncertainty for physics-based models. The first part of this presentation will focus on the following topics in forward UQ:

- Sensitivity analysis
- Monte Carlo sampling methods
- Response surface approximations
- Multi-level and multi-fidelity methods

Most of these methods are available in open-source toolkits, such as Dakota [1]. The second part of the presentation will focus on the following topics in inverse UQ:

- Ill-posedness in deterministic and stochastic inverse problems
- Bayesian formulations for parameter estimation [2]
- Consistent formulations for stochastic inversion [3]
- Optimal experimental design [4]

Numerical examples using physics-based models will be given throughout the presentation to demonstrate each of the methods/concepts.

1. Adams, B.M., Bauman, L.E., Bohnhoff, W.J., Dalbey, K.R., Ebeida, M.S., Eddy, J.P., Eldred, M.S., Hough, P.D., Hu, K.T., Jakeman, J.D., Stephens, J.A., Swiler, L.P., Vigil, D.M., and Wildey, T.M., "Dakota, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 6.0 User's Manual," *Sandia Technical Report* SAND2014-4633, July 2014. Updated November 2015 (Version 6.3).
2. Stuart, A. M., "Inverse problems: A Bayesian perspective", *Acta Numerica*, 19 (2010).
3. Butler, T., Jakeman, J., and Wildey, T. "Combining push-forward measures and Bayes' rule to construct consistent solutions to stochastic inverse problems". *SIAM Journal on Scientific Computing,* 40:2 (2018).
4. Huan, X., and Marzouk, Y. M. "Simulation-based optimal Bayesian experimental design for nonlinear systems". *Journal of Computational Physics* 232, 1 (2013).