Data Management and Uncertainty Quantification for EPSI

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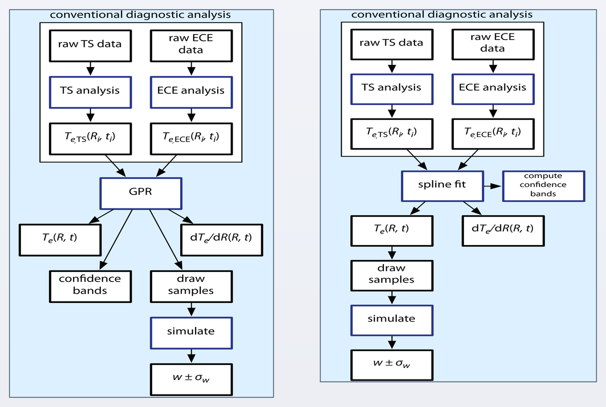
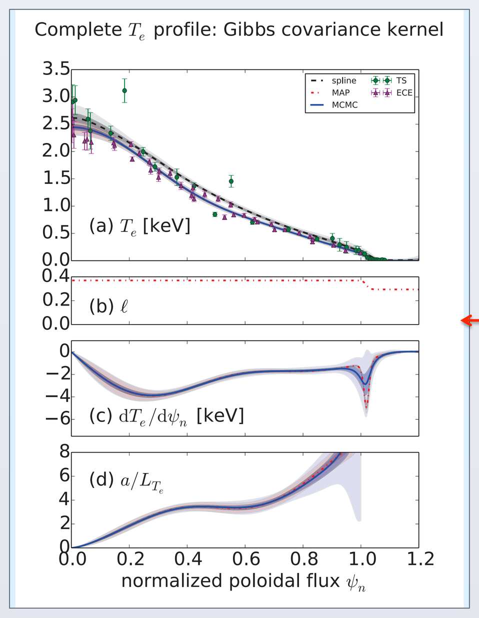
Uncertainty Quantification

Improved Profile Fitting and UQ using Gaussian Process Regression(MIT)[1]

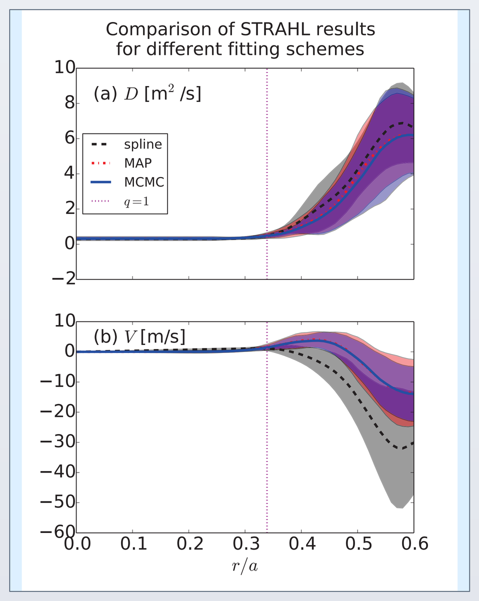
- EPSI Codes need UQ analyzed experimental data for reliable validation
- Fitting of smooth profiles from discrete observations key plasma simulation input
- Existing spline fitting techniques have deficiencies
- Gaussian Process Regression(GPR) captures existing results while delivering
  - Statistically rigorous fits for plasma profiles and gradients(key XGC1 inputs)
  - Uncertainty estimates for key plasma profiles and gradients
  - Increased convergence rate of forward uncertainty propagation
  - Implementation general and widely applicable.

Spline vs GPR fitting Workflows





Profile fitting for T_e(electron temperature) from Thomson Scattering (TS) and electron cyclotron emission(ECE) system data. GPR results shown using maximum a posteriori(MAP) and Markov Chain Monte Carlo(MCMC) approaches. Error bars and dark shading is ±σ, light shading ±3σ.

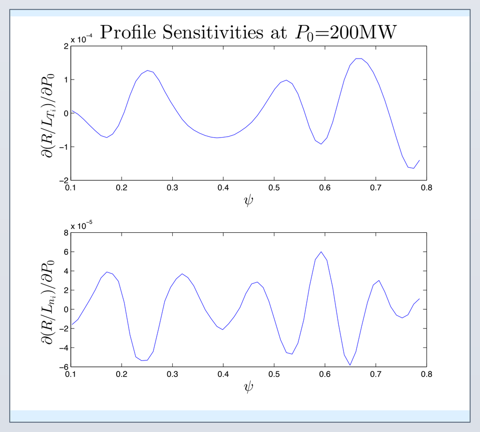


STRAHL takes electron profiles and initial guesses on impurity transport coefficients D and V and iterated to match exp. data. D and V are highly sensitive to profile uncertainties. The uncertainty envelopes are ±σ.

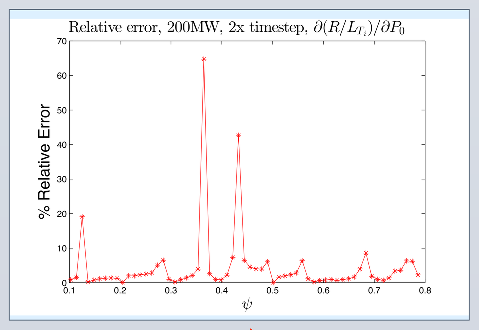
[1] M A Chilenski, M Greenwald, Y Marzouk, N T Howard, A E White, J E Rice, and J R Walk (MIT), submitted to Nuclear Fusion, work supported under cooperative agreement C-Mod: DE-FC02-99ER54512

Sensitivity of Plasma Gradients in XGC1 to Applied Heating(UTexas,PPPL)[2]

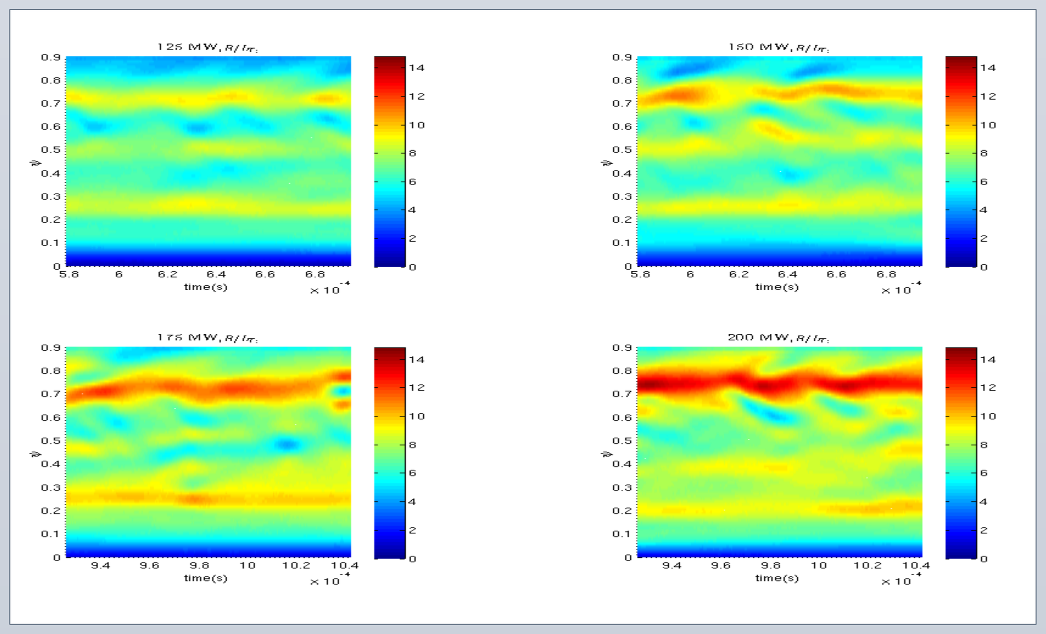
- Complete UQ workflow involves characterization of input uncertainties (see above), forward propagation via XGC1, and comparison of quantity of interest(QoI) (often via synthetic diagnostic) with experimental data.
- Uncertainties in model input parameters (λ) may impact QoI. Many parameters-intractable sampling problem given the cost of global gyrokinetic simulation.
- Goals of Sensitivity Analysis(SA):
  - Potentially reduce size of input space to be sampled by removing unimportant parameters *(Reduce # of simulations for UQ)*
  - Characterize effect of numerical parameters (grid, particle count, timestep) on QoI (plasma profiles) *(Reduce cost of simulations for UQ)*
  - Quantify effects of embedded physics models on QoI *(Reduce cost of simulations)*
- Motivated by our goal of studying L-H transition and nonlocal edge effect on core, we are performing a SA of plasma profiles to a heating model. We are using a combination of sampling approaches to compute dQoI/dλ.
- Moderate case (CYCLONE base case) allows sensitivity computations at lower cost.
- Sensitivity predictions combined with scaling studies will be compared against larger scale, enriched physics XGC1 runs: Use reduced system to project UQ of full system
- Repeat process with enriched physics, increased problem size if extrapolation*(combined with input uncertainties)* is invalidated by new simulation data.



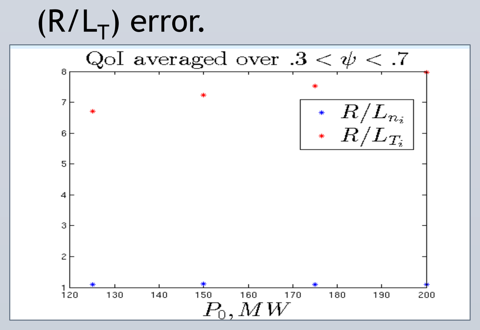
"Steady-state" gradient sensitivities computed at 200MW; temperature (naturally) more sensitive than density.



Attempt to coarsen timestep(2x) (4x timestep unstable at 200MW) led to marginal accuracy results(Mean error=4.42%), with even worse results for profile (R/L_T) error.



Different applied heating powers lead to differing simulation times to steady state.125MW, 150 MW are near steady state, while 175MW, 200MW are not. Expected monotone behavior in P_0 of R/L_T is observed. Quantifying acceptable level of "steady-state" variation is governed by the QoI.



Expected behavior of T, n profiles under P_0 scaling; density QoI stiff and reaches steady state quickly.

[2] Simulations performed at NERSC on Edison.

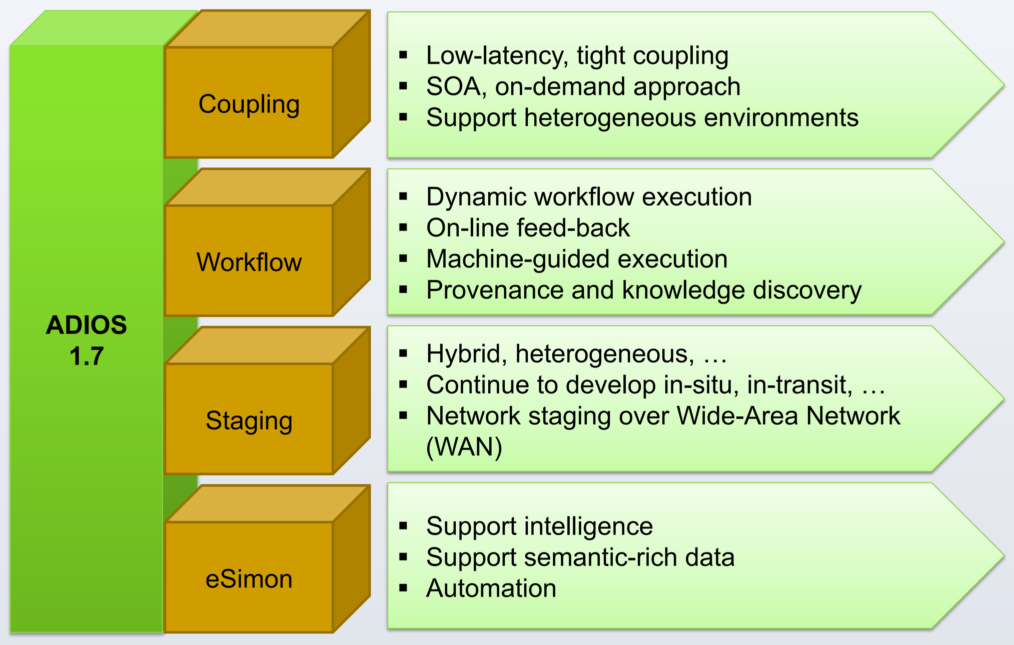
Calibration of XGCa Anomalous Diffusion under Uncertainty(UTEXAS,MIT,PPPL)

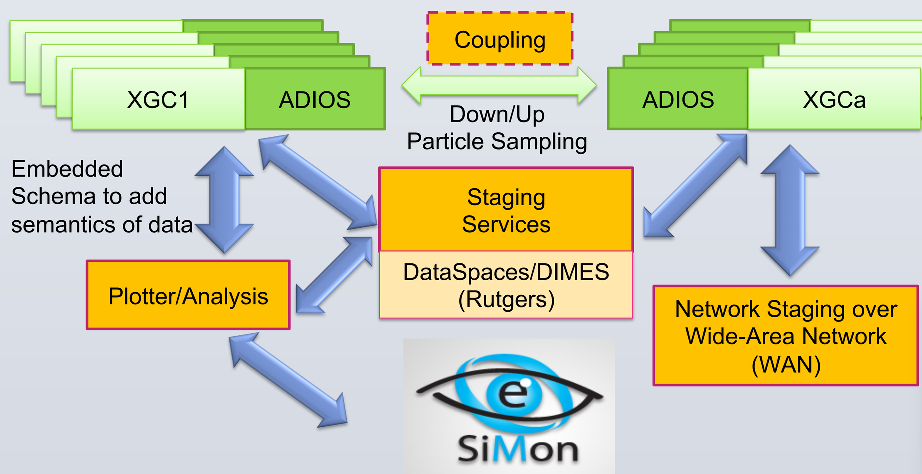
- Following D.Battaglia et al(2014), we are performing a calibration of an anomalous diffusion model.
  - Calibration will be Bayesian, using SCIDAC QUEST center software QUESO.
  - Plan to use Alcator CMOD data to calibrate model in a variety of modes relevant to L-H transition.
  - May use high-fidelity XGC1 simulation results as additional calibration training data.
  - Will examine use of XGCa+calibrated model as a surrogate for XGC1 sensitivity analysis.

Data Management

ADIOS (2013 R&D 100 winner. Current version 1.7) has been integrated with EPSI simulations to support:

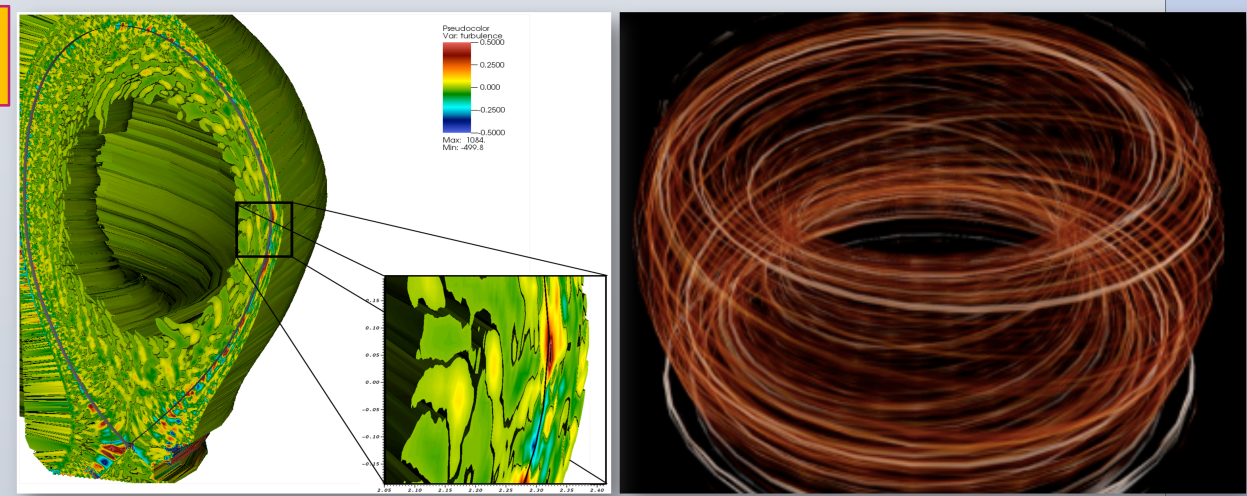
- Data staging with low-latency, tight coupling execution environments through in-memory data exchanges between different codes.
- Service Oriented Architecture (SOA) for on-demand coupling executions with support of dynamic workflow invocation.
- Coupling executions in heterogeneous computing environments with streaming data support. Network staging over Wide Area Network (WAN) under development.
- Selection and chunked reads to enable schedule optimization.





Data-centric integrated execution environment

Our focus is to support EPSI simulation by providing integrated data-centric execution environments for tight code coupling, staged data process, and monitoring system with a support of dynamic workflow system.

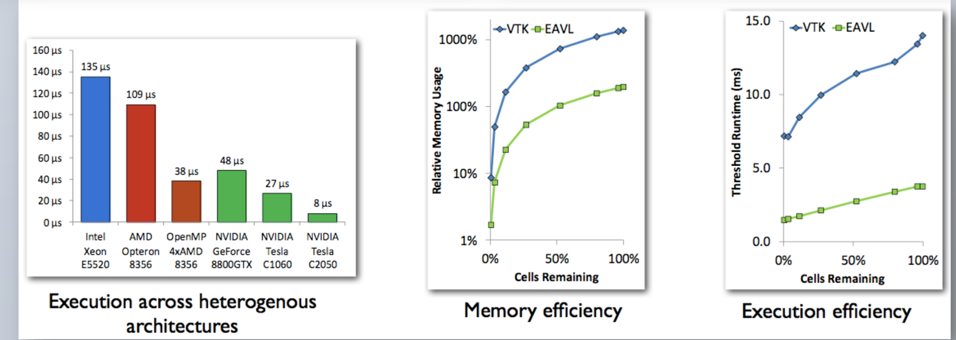


ADIOS Vis Schema

- Create an easy-to-use schema for ALL ADIOS codes.
- Facilitates data sharing without adding code complexity, or slowing down the code.
- Visualization schema: Semantics of the data for the purpose of visualization.
- Describing visualization data for various tools (VTK, Matlab, ParaView).

Future of XGC Reader

- Support for ADIOS Vis Schema.
- Filtering of turbulence.
- Integration with higher quality rendering with visualization software from OLCF.

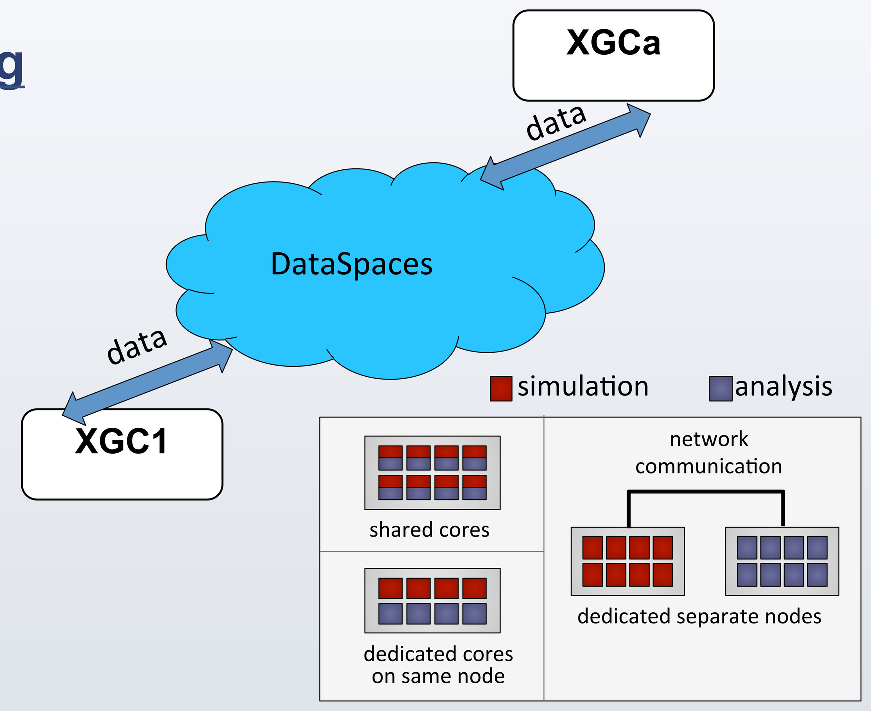


EAVL: Extreme Scale Analysis and Visualization Library

Data Staging

EPSI coupling workflow

- Goal: To enable tightly coupled XGC1 and XGCa workflow using memory to memory coupling for experimental time scale simulation



DataSpaces As a Service

- Persistent staging servers run as a service.
- Coupled applications can join, progress and leave independently.
- New approach targets more complex workflows and provides more flexibility.
- DataSpaces As a Service will improve resource efficiency and increase I/O performance.

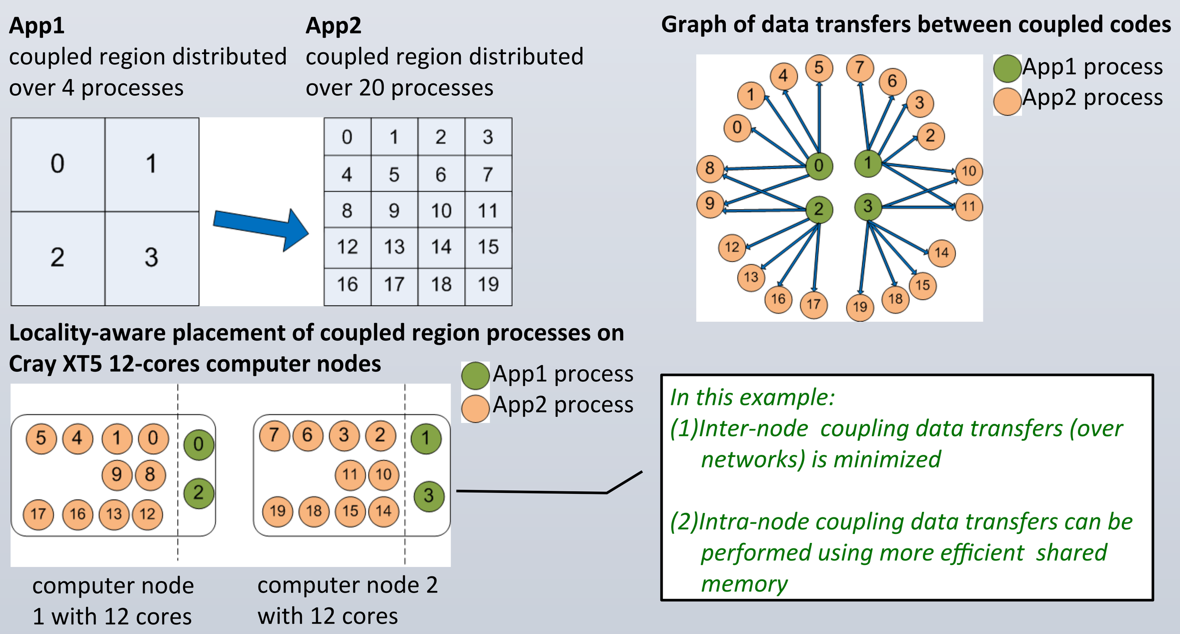
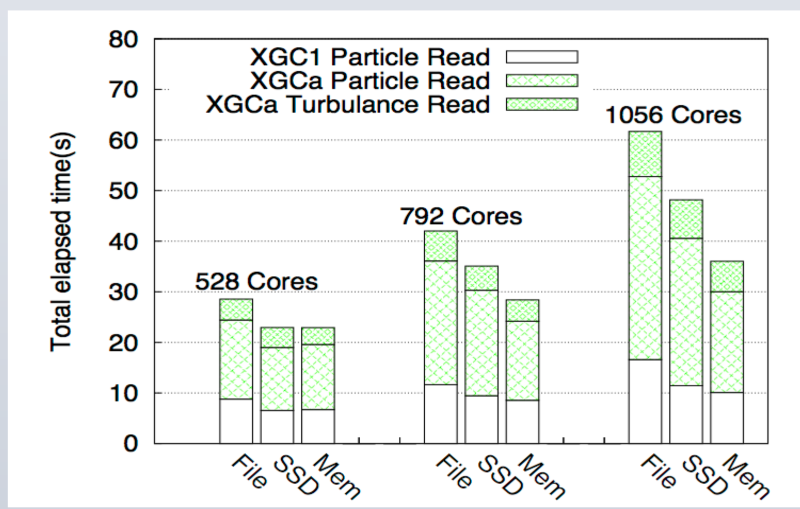


Illustration of the data-centric mapping of the application process for concurrently coupled workflow



Preliminary Result

- Enable exchange data through on-node memory.
- Data locality and core-level parallelism can be exploited to reduce data movement by increasing intra-node data sharing.
- Utilize SSD for data bursting.