SAND2021-8872C

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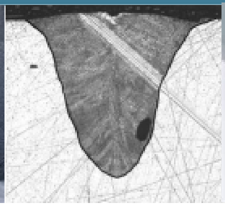
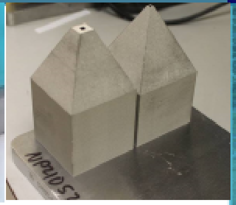
Rapid Computation of Thermal Histories for Laser Powder Bed Fusion Additive Manufacturing Processes





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USNCCM 16

July 27, 2021

U.S. DEPARTMENT OF ENERGY NNSA

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Background

- Laser Power Bed Fusion (LPBF) is seeing increasing use as a technology for producing functional parts
- Wanted: End-to-end modeling of LPBF process to predict part performance
  - Reduce experimental workload
  - Inform process design and qualification
  - Stand up new materials/machines/processes
- Fully resolved build predictions remain largely intractable, causing reliance on phenomenological models
  - Inherent strain
  - Agglomeration
- Presented here: Green's function technique for fully time-resolved part-scale thermal predictions

Green's Function

- Analytical Green's function solution exists for linear, 3D, time-dependent heat equation
- Analytical spatial integral
- Solution via 1D numerical integral
- **Embarrassingly parallel!**
- Previous AM applications:
  - Wolfer et al (Add. Manuf. 2019)
  - Farwell et al (FEF 2019)
- Full part thermal histories achieved here through use of 4D adaptive grids

Green's function:

$$G = H(t-s)\left(\frac{1}{4\pi\alpha(t-s)}\right)^{\frac{3}{2}} e^{-\frac{(x-x')^2+(y-y')^2+(z-z')^2}{4\alpha(t-s)}}$$

Ellipsoidal Gaussian:

$$Q = \frac{P}{\pi^{3/2}\sigma_x\sigma_y\sigma_z} e^{-\frac{(x-x_l)^2}{\sigma_x^2}-\frac{(y-y_l)^2}{\sigma_y^2}-\frac{(z-z_l)^2}{\sigma_z^2}}$$

Temperature Solution:

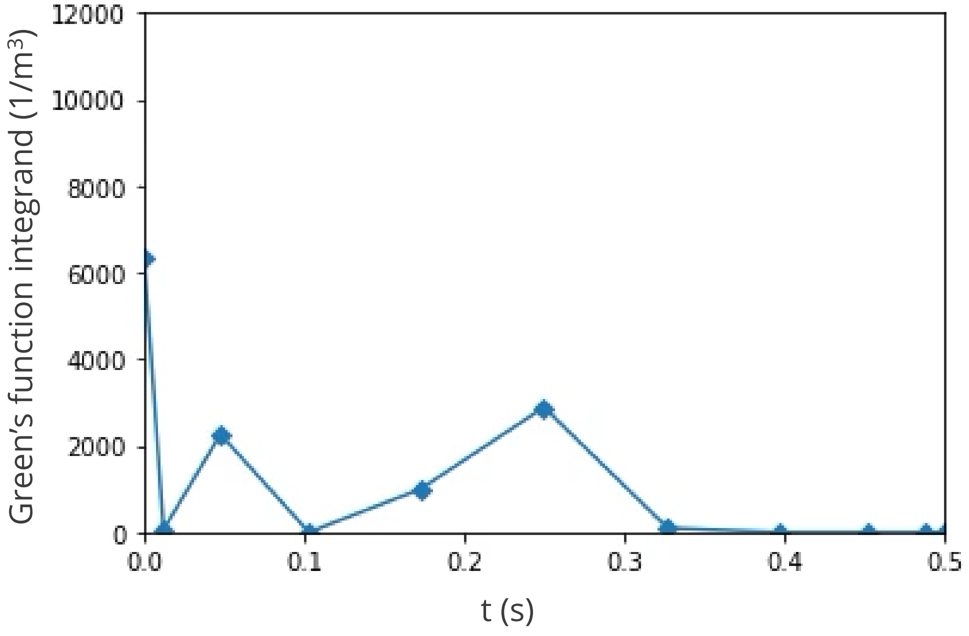
$$T_i + \frac{2P}{\pi^{3/2}\rho c}\int_0^t \frac{\exp\left\{-\frac{(x-x_l(s))^2}{\sigma_x^2+4\alpha(t-s)}-\frac{(y-y_l(s))^2}{\sigma_y^2+4\alpha(t-s)}-\frac{(z-z_l)^2}{\sigma_z^2+4\alpha(t-s)}\right\}}{\sqrt{\sigma_x^2+4\alpha(t-s)}\sqrt{\sigma_y^2+4\alpha(t-s)}\sqrt{\sigma_z^2+4\alpha(t-s)}}ds$$

Assumptions:

- Material properties k, ρ, c do not depend on T, x, y, z, or t
- Domain is semi-infinite

Methodology

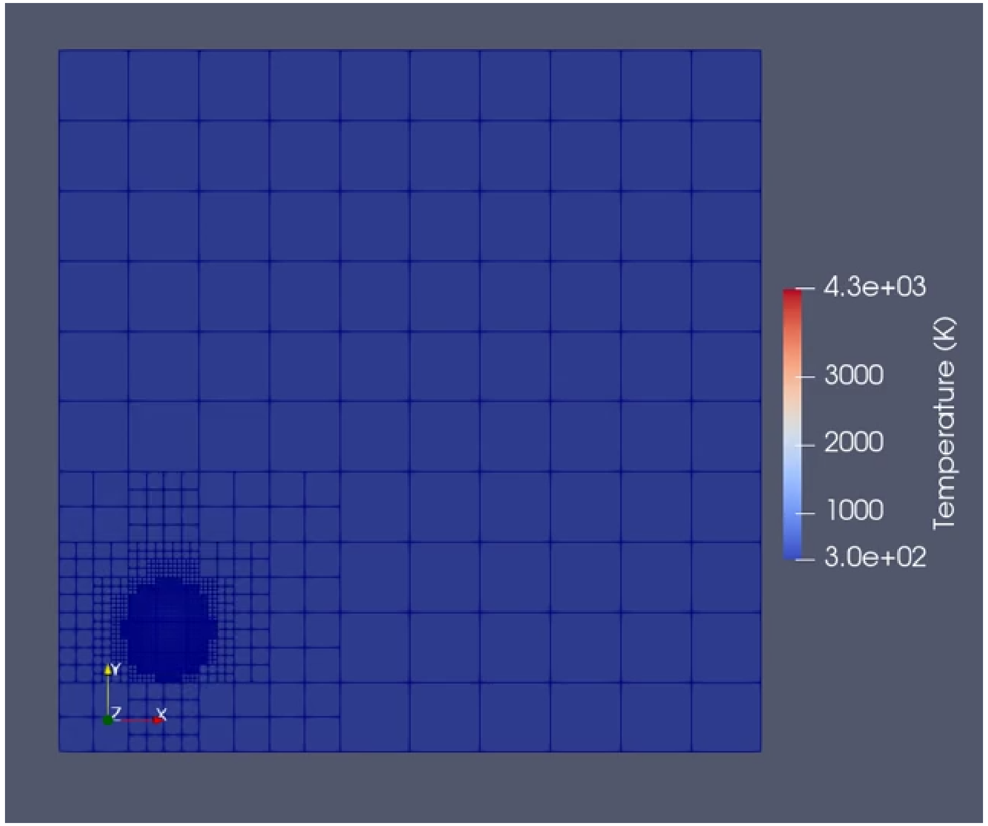
- Piecewise linear discretization of laser source
- Numerical integration via adaptive Clenshaw-Curtis quadrature
  - Nested quadrature orders with adaptive interval splitting
  - Efficient integration of highly localized integrand over long time intervals
- Time-parallel computation of each layer
- Fully time resolved laser action
- Implemented on CPU and GPU using Kokkos



Adaptive integration of Green's function for a point

Adaptive Space-Time Grid

- Independent T evaluations decouple resolution and accuracy
  - Initial coarse sampling on uniform grid
  - Refine each space-time cell
  - Cell-by-cell evaluation of interpolated and actual fine solution
  - Further refine cells where interpolant is inaccurate
- CPU/GPU mesh adaptivity
- Compact(ish) solution representation
- Decomposition with **no communication across ranks**



Adaptive 4D Grid projected onto 3D mesh

Comparison to FEM

- Benchmark problem: square scan pattern
  - 0.6s of simulated time
  - 10μm x 100μs resolution
- 12x/72x speedup on CPU/GPU
  - CPU comparison is equal # of procs
  - Green's function method effectively scales to many more procs
- 84GB vs 4.5TB (uncompressed) to represent solution on adaptive space-time grid vs fixed resolution

Solver	Platform	# Procs	Time
FEM	CPU	360	6 hrs
Green	CPU	360	33 mins
Green	GPU	16	4.3 mins

Full Build

- Full size (big) part
  - 5x5x10cm
  - 3086 layers
- Time resolved solution intractable with FEM
- **~3 days on 2400 CPU processes**
  - No large enough GPU cluster!
- Approx. 100TB of data (compressed)
  - File writes/compression significant cost
  - More compact representation needed

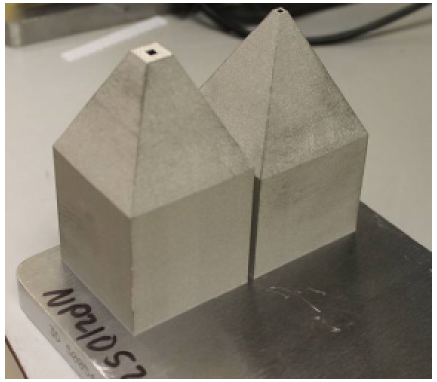
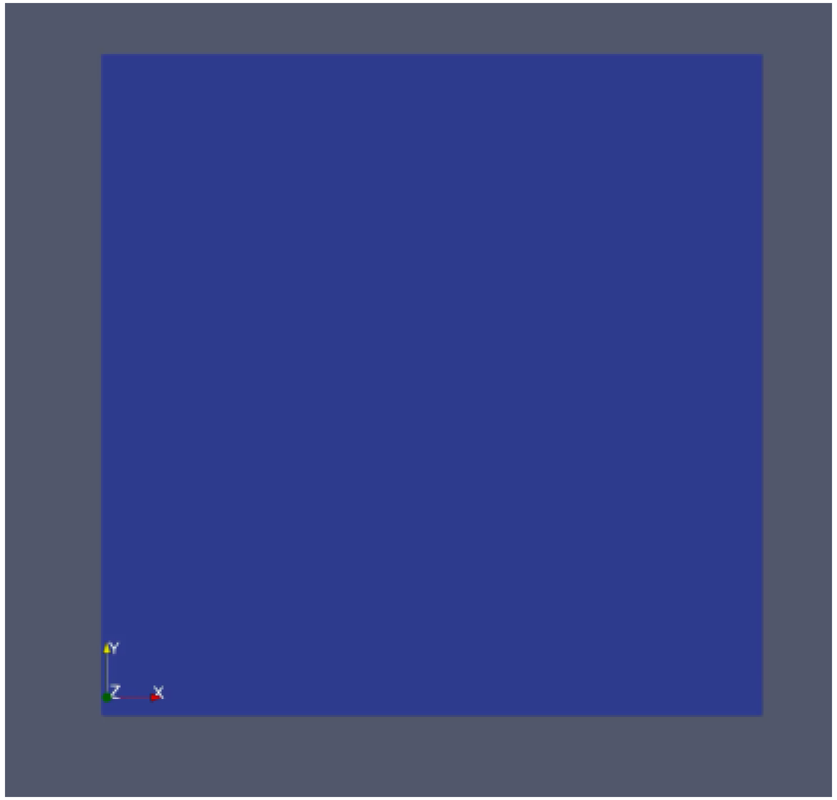


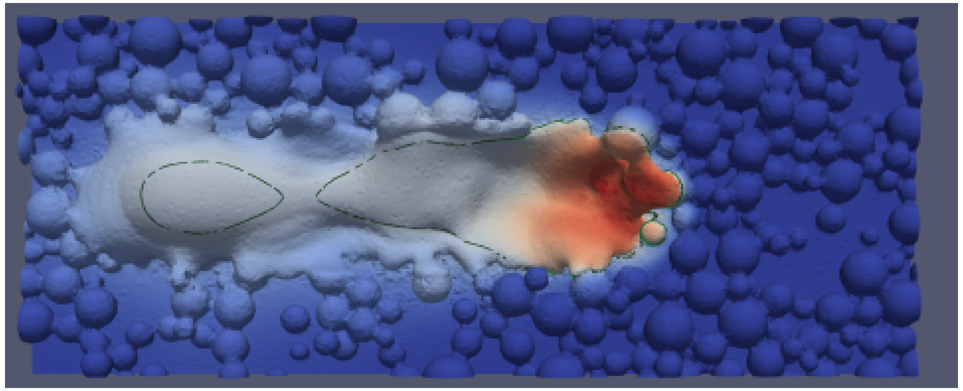
Photo of simulated part



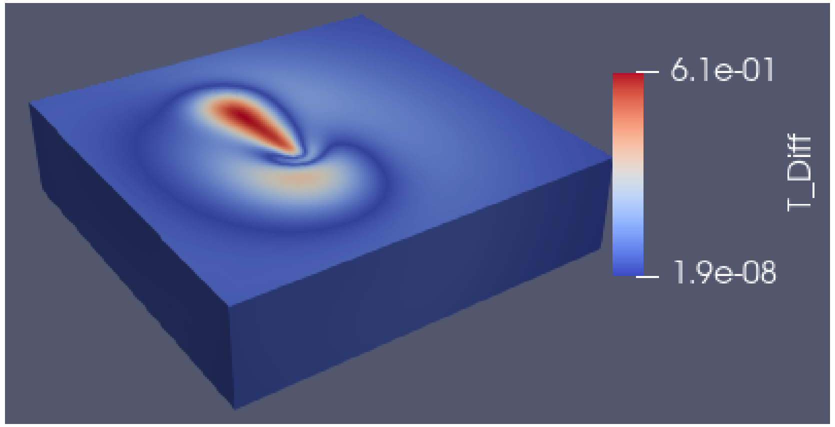
Temperature history of a full layer scan

Calibration/Temperature Comparisons

- Linear model can be calibrated to match desired melt pool dimensions
  - Non-linear conduction models, thermal/fluid models, experimental data
- L1/L2 temperature norm calibration
- Differences in temperature history regardless of method
  - Non-linear heat capacity effects in trailing edge of melt pool
- Multi-grid Jacobi-type methods to iterate out non-linearities and complex BCs
- Model form uncertainty quantification



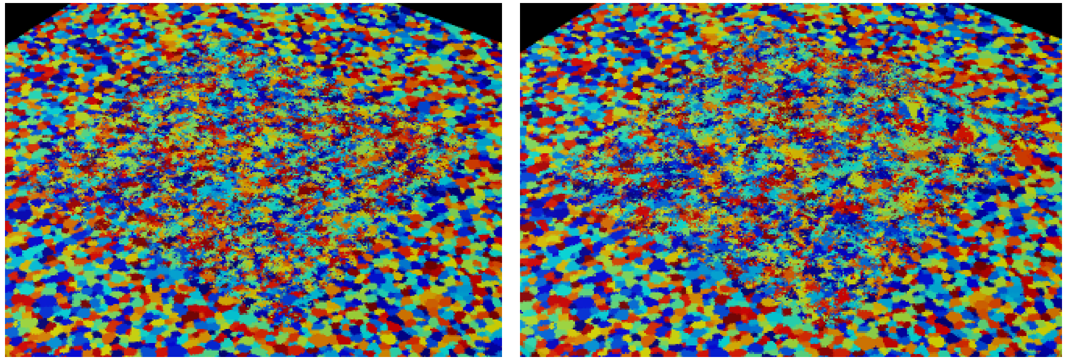
Melt pool simulated using mesoscale thermal/fluid model



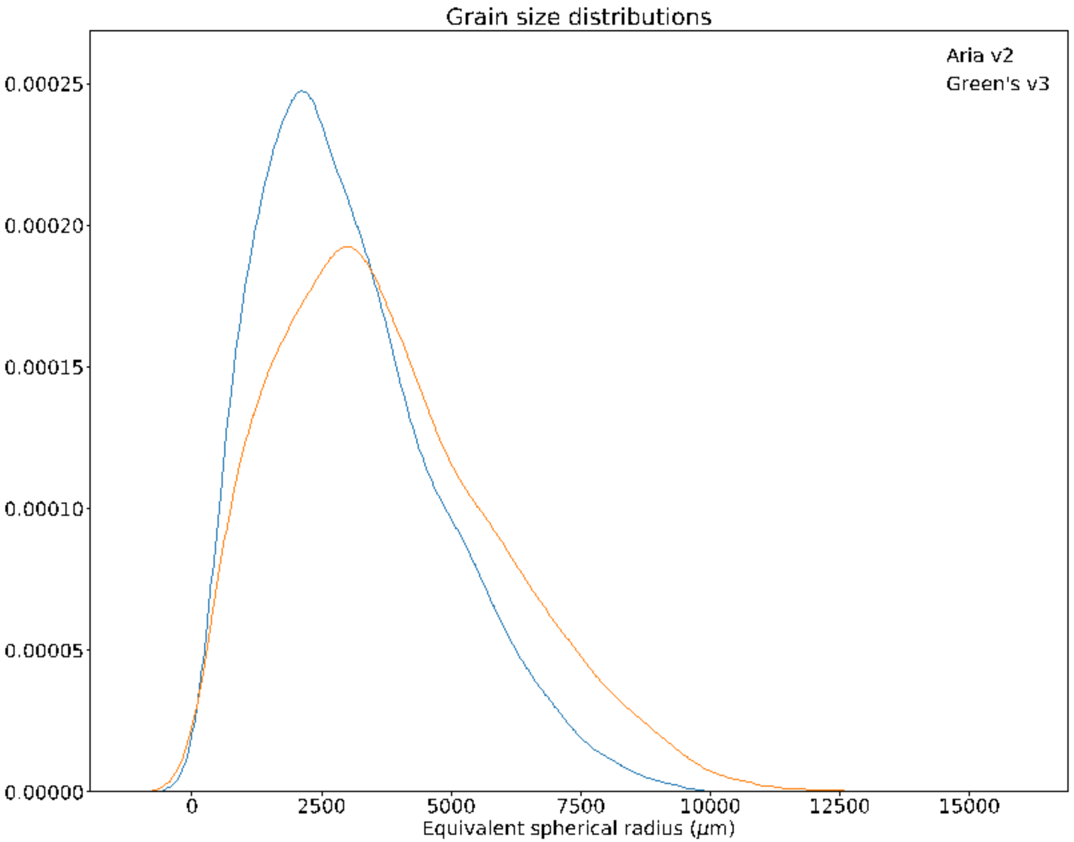
Normalized temperature difference between calibrated linear and non-linear models

Microstructure Comparisons

- Both models show fine grain structures
  - Small melt pool w/limited remelting
- Linear Green's results show shift towards larger grain sizes
  - Differences in thermal gradients due to latent heat/variable specific heat



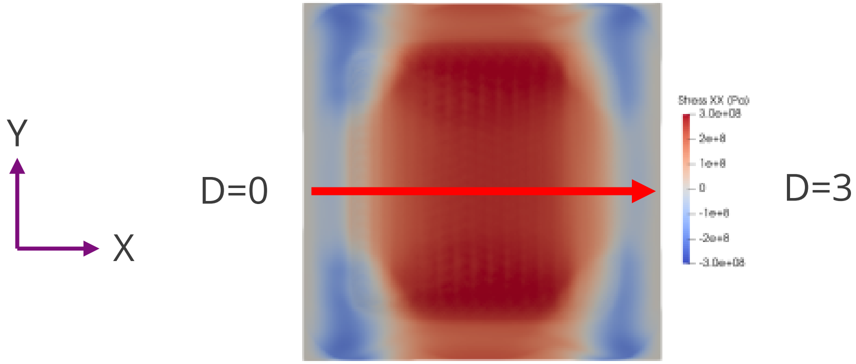
Comparison of microstructures computed for single layer using (a) non-linear and (b) linear thermal models



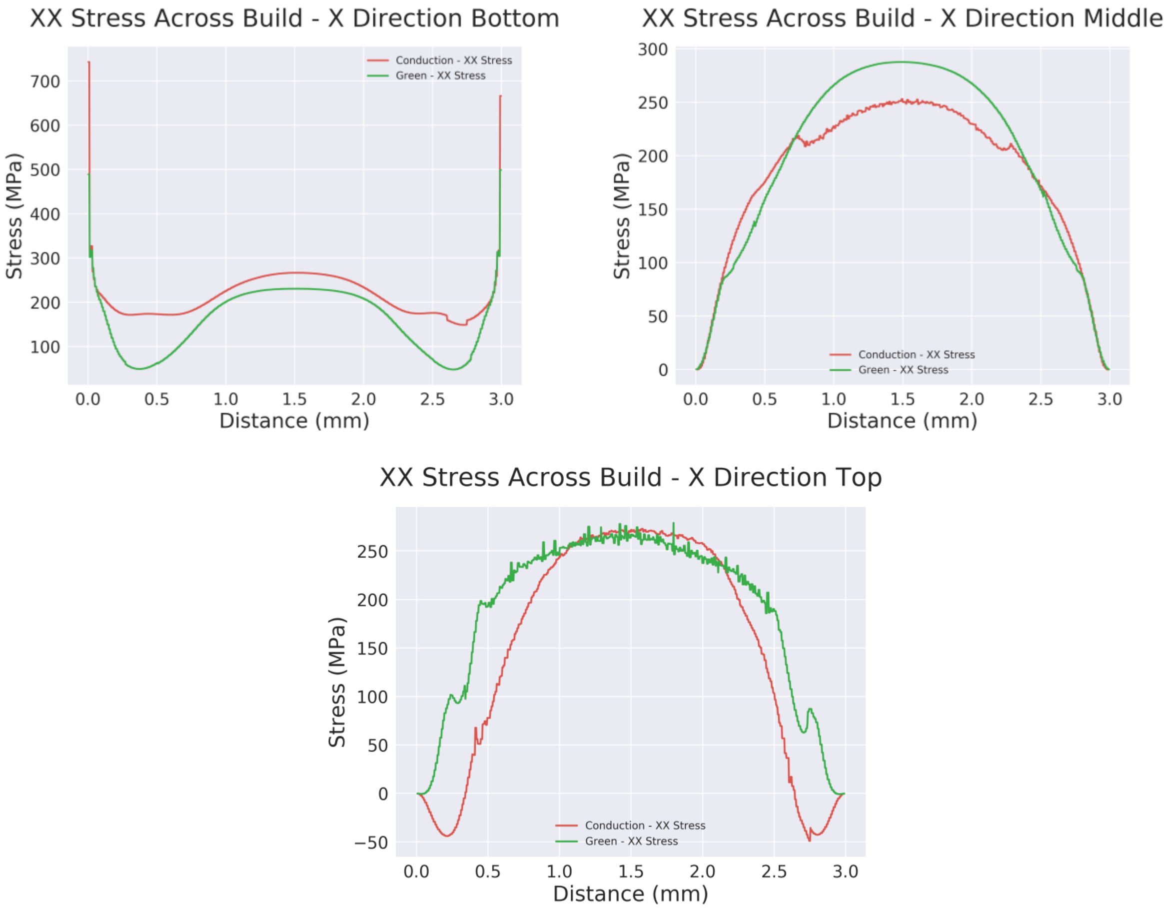
Equivalent spherical radius grain populations for non-linear (blue) vs linear (brown) temperature histories

Residual Stress Comparisons

- Agreement in part interior is good
- Biggest differences at edges
  - Different applied BCs
- Temperature differences don't always translate to large stress or microstructure differences



Location of residual stress line contours



Comparisons of XX residual stress perpendicular to scan direction at three different depths

Conclusions

- Green's function solver implemented
  - Highly parallel
  - CPU/GPU capable
  - CPU/GPU adaptive 4D grid
  - 12x/72x CPU/GPU speedup vs FEM
- **Fully time resolved large (5x5x10cm) part build in ~3 days**
- Future work
  - Compact data representation
  - Resolve non-linearities, complex BCs
  - **Uncertainty estimation**