Scaling PDE Solvers to Exascale

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NekCEM, NekLBM, Nek5000: Scalable Software based on Spectral-Element Discretizations for Electromagnetics and Fluids

- **Peta- and exascale simulations are driven by scale disparity: small scales λ interacting with scales L>> λ**
- **Dispersion errors accumulate linearly with time:**

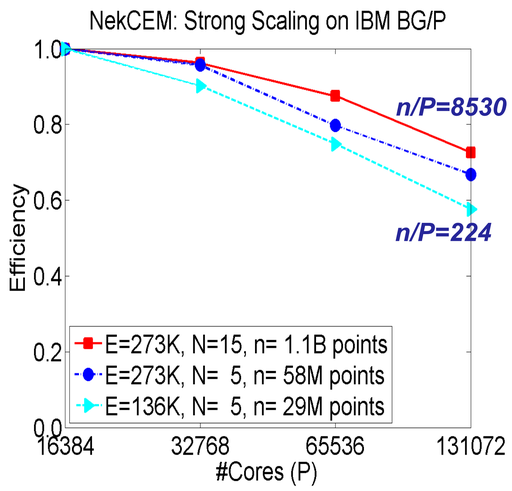
  ε_t ~ |correct speed – numerical speed| * t

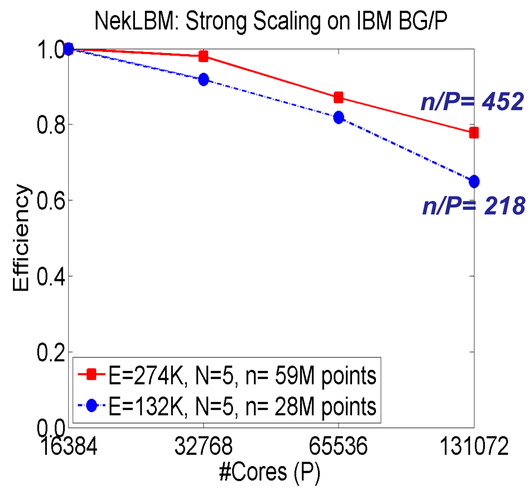
  → ε_{final} ~ |numerical dispersion error| * t_{final}

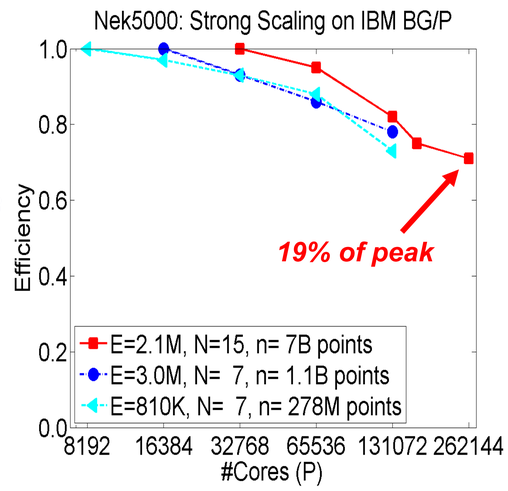
  ~ |numerical dispersion error| * (L/λ)
- **For final error** $\varepsilon_{final} < 1$, **require:**

  |numerical dispersion error| ~ $(\lambda/L)\varepsilon_{final} \sim O(h^N) << 1$

  h: grid spacing, *N*: approximation order
- **Well-implemented, high-order discretizations efficiently deliver small dispersion errors, yielding an *order-of-magnitude* savings in computational cost (Kreiss & Oliger 72, Gottlieb et al. 07)**







High-Order Simulation Codes

- **NekCEM: Computational electromagnetics**

  Key Features: Spectral element discontinuous Galerkin (SEDG) with explicit timestepping

  Open source with excellent scaling *to P=131,072* cores, even at fine granularity *n/P~200*

  Vector communication: 1 message for 6 fields

  Scalable I/O tested to *P=65,536* with 5 seconds to write a single snapshot for a 1 billion-point

  Current capability: Wakepotential calculations for beam dynamics; Nano SERS simulations

  Future applications: Ultrashort beam simulations for the ILC, Electron transport simulations for solar cells, Nanoscale materials optimization in the presence of uncertainty
- **NekLBM: Incompressible/Compressible/Multiphase flows**

  Key Features: SEDG lattice Boltzmann method (LBM) with explicit timestepping

  Splitting steps for collision and streaming, based on the 9-, 13- and 19-velocity lattices

  Open source with excellent scaling *to P=131,072* cores, even at fine granularity *n/P~200*

  Vector communication: 1 message for 9, 13, and 19 fields

  Current capability: Single phase flows modeling (in comparison to SE and vortex methods)

  Future applications: Water reactor modeling with scalable algorithms for multiphase flows
- **Nek5000: Fluid mechanics, Heat transfer, MHD, Combustion**

  Key Features: Advanced iterative solvers (including scalable coarse-grid solver); Open source, ~100 users, > 200 publications

  Scales to > *P=260,000* cores (1999 Gordon Bell Prize)

  Full feature support – e.g., scalable communication kernels, parallel interpolation – many of which have been integrated into other DOE codes.

  Parallel efficiency: > 70% on *P=262K*, 7 billions points (tests $n > 2^{31}$)

  > 83% on *P=131K*, for *n/P ~ 6200*, *E=810,000*, *N=9*

  > 73% on *P=131K*, for *n/P ~ 3100*, *E=810,000*, *N=7*
- **Future Plan:**

  Address SE multigrid for new flow discretizations

  Monotone preserving schemes for scalar transport

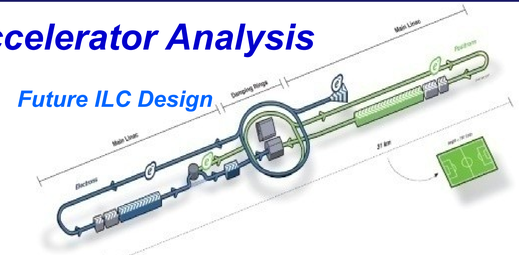
  Scalable Schrödinger-Poisson solver for electron transport

  Vlasov solver for particle beam dynamics

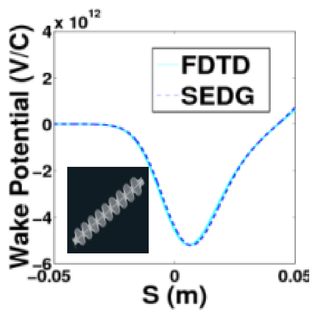
  Hybrid MPI/OpenMP/Pthread programming to exascale for multicore nodes

Accelerator Analysis

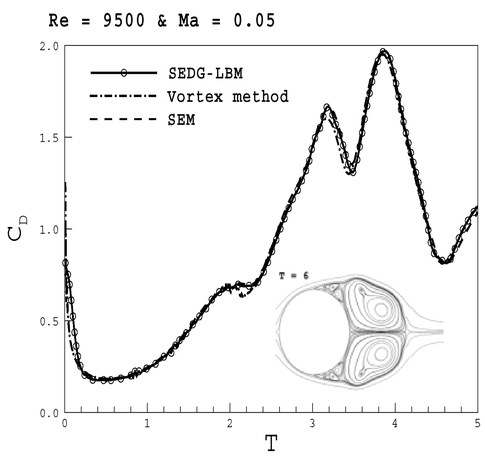
Future ILC Design



TESLA cavity

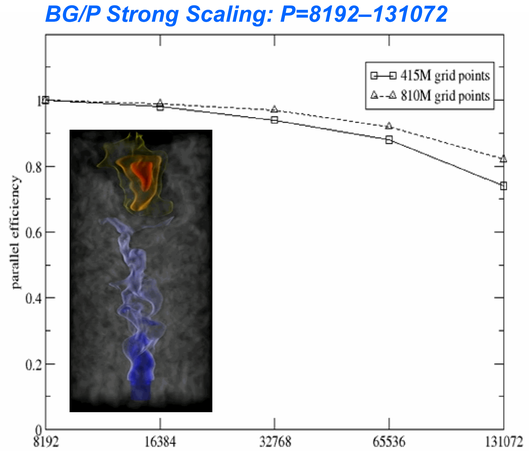


Lattice Boltzmann Method



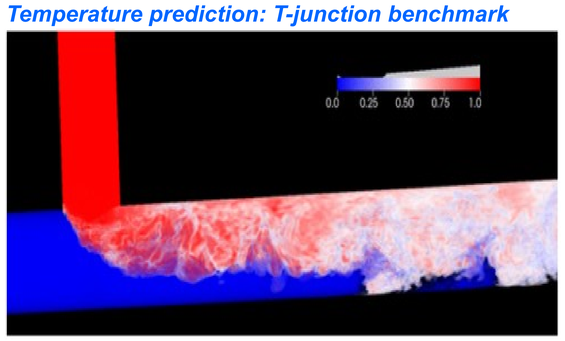
Turbulent Combustion

BG/P Strong Scaling: P=8192–131072

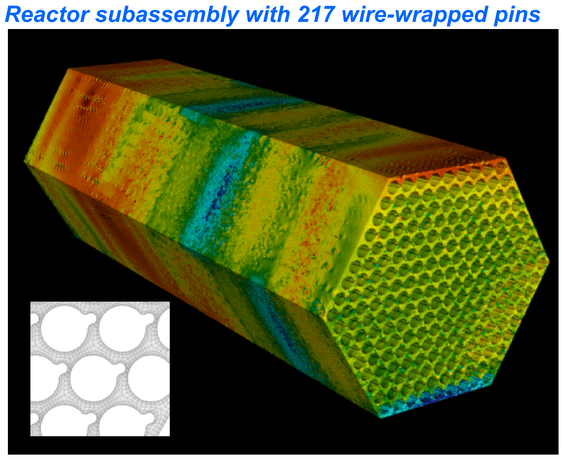


Nuclear Reactor Modeling

Temperature prediction: T-junction benchmark

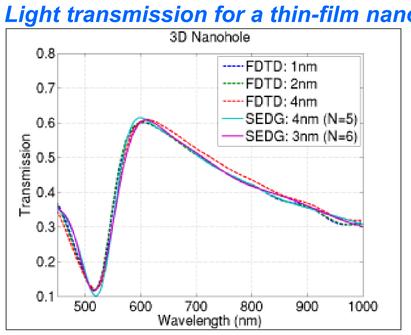


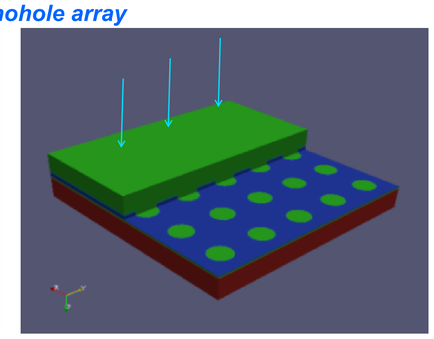
Reactor subassembly with 217 wire-wrapped pins



Nanophotonics

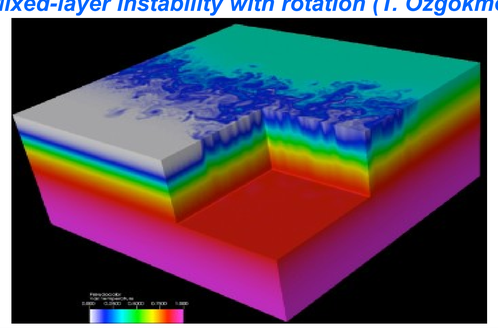
Light transmission for a thin-film nanohole array





Ocean Modeling

Mixed-layer instability with rotation (T. Ozgokmen)



Supported by the Mathematical, Information, and Computational Sciences Division of the Office of Advanced Scientific Computing Research, Office of Science, and by the Nuclear Energy program, U.S. Department of Energy. Computational resources provided by a grant from the DOE Office of Science INCITE program.