Quinoa: Adaptive Computational Fluid Dynamics

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https://github.com/quinoacomputing/quinoa

Goal: hardware-adaptive large-scale multiphysics

- Fluid dynamics, turbulence, particle transport, chemistry, plasma physics of non-ideal multiple mixing materials
- Automatic dynamic computational load redistribution for real-world problems
- Preserving the domain scientist's sanity

Agenda:

- Philosophy
- Infrastructure
- Two tools: particle solver, unstructured-grid PDE solver
- Future plan

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Philosophy

- Partition everything
- Be asynchronous everywhere
- Automate everything
- Remember that everything fails

Strategy

- Most physics codes start with capability *then* software engineering is an afterthought
- We start with a state-of-the-art production code *then* put in physics
- From scratch: *not* based on existing code
- C++11 & Charm++ (fully asynchronous, distributed-memory parallel)

Funding & history

- Started as a hobby project in 2013 (weekends and nights)
- First funding: Oct 2016

Work in progress

Infrastructure

- 46K lines of code
- 20+ third-party libraries, 3 compilers
- Unit-, and regression tests
- Open source: `https://github.com/quinoacomputing/quinoa`
- Continuous integration (build & test matrix) with Travis & TeamCity
- Continuous quantified *test code* coverage with Gcov & CodeCov.io
- Continuous quantified *documentation* coverage with CodeCov.io
- Continuous static analysis with CppCheck & SonarQube
- Continuous deployment (of binary releases) to DockerHub

Ported to Linux, Mac, Cray (LANL, NERSC), Blue Gene/Q (ANL)

Current tools

1. *walker* – Random walker for stochastic differential equations
2. *inciter* – Partial differential equations solver on 3D unstructured grids
3. *rngtest* – Random number generator test suite
4. *unittest* – Unit test suite
5. *meshconv* – Mesh file converter

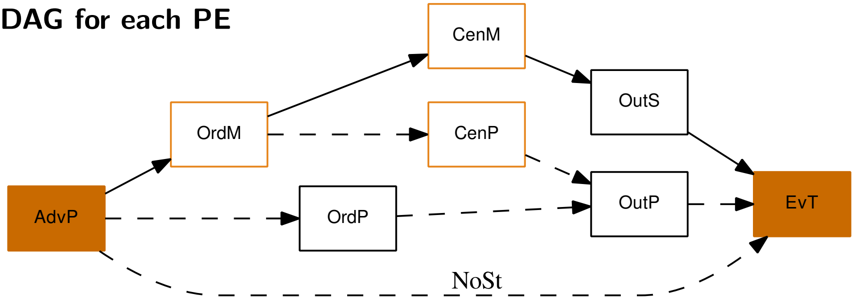
Quinoa::Walker

- Particle solver
- Numerical integrator for stochastic differential equations
- Used to analyze and design the evolution of fluctuating variables and their statistics
- Used in production for the design of statistical moment approximations required for modeling mixing materials in turbulence
- **Future plan:** Predict the probability density function in turbulent flows

$$\frac{\partial}{\partial t}F(\mathbf{Y},t) = -\sum_{\alpha=1}^{N-1}\frac{\partial}{\partial Y_\alpha}\left[A_\alpha(\mathbf{Y},t)F(\mathbf{Y},t)\right] + \frac{1}{2}\sum_{\alpha=1}^{N-1}\sum_{\beta=1}^{N-1}\frac{\partial^2}{\partial Y_\alpha \partial Y_\beta}\left[B_{\alpha\beta}(\mathbf{Y},t)F(\mathbf{Y},t)\right]$$

$$\mathrm{d}Y_\alpha(t) = A_\alpha(\mathbf{Y},t)\mathrm{d}t + \sum_{\beta=1}^{N} b_{\alpha\beta}(\mathbf{Y},t)\mathrm{d}W_\beta(t), \qquad \alpha = 1,\dots,N, \qquad B_{\alpha\beta} = b_{\alpha\gamma}b_{\gamma\beta}$$

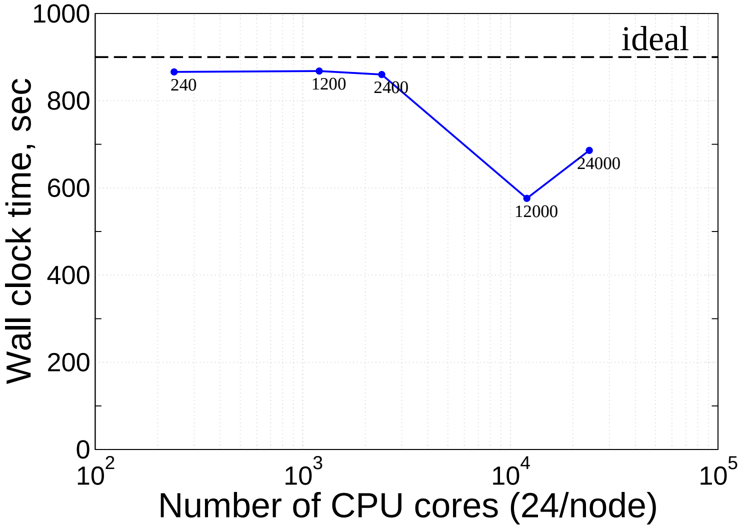
Walker SDAG for each PE



AdvP – advance particles
OrdM – estimate ordinary moments
CenM – estimate central moments, e.g., $\langle y - \langle Y \rangle \rangle^2$
OutS – output statistical moments
EvT – evaluate time step
OrdP – estimate ordinary PDFs
CenP – estimate central PDFs, e.g., $F(y - \langle Y \rangle)$
OutP – output PDFs
NoSt – no stats, nor PDFs

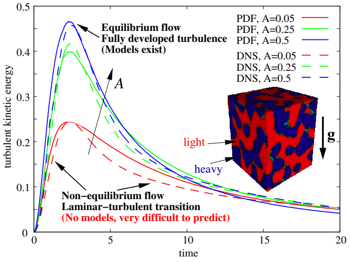
src/Walker/distributor.ci

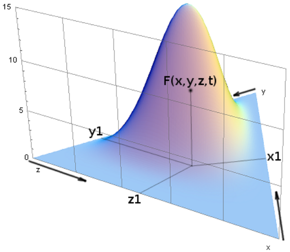
Walker weak scaling with up to 3x10^9 particles

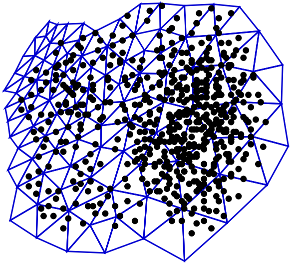


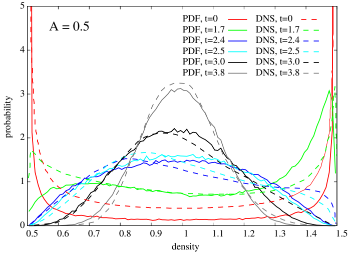
Quinoa::Walker future plan

- **Goal:** Predict the probability density function in turbulent flows
- **Why:** Because it requires less approximations
- **How:** Integrate a large particle ensemble governed by stochastic differential equations
- The ensemble represents the fluid itself
- Statistics and the discrete PDF extracted from the ensemble in cells







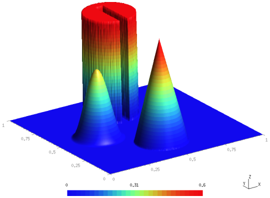


Quinoa::Inciter

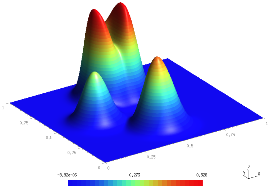
- PDE solver for 3D unstructured (tet-only) grids
- Native Charm++ code using MPI-only libs: *hypre*, *Zoltan2*
- Simple Navier-Stokes solver for compressible flows
- Finite elements
- Flux-corrected transport
- Asynchronous linear system assembly
- File/PE I/O
- Current work: adaptive mesh refinement, V&V
- **Future plan:** use AMR to explore scalability with large load-imbalances

Flux-corrected transport

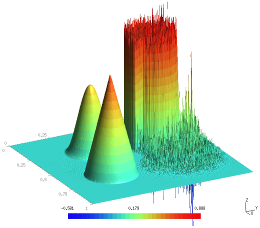
- Used when stuff (e.g., energy) moves from A to B (i.e., all the time)
- Godunov theorem: No *linear* scheme of order *greater than one* will yield *monotonic* (wiggle-free) numerical solutions.
- A solution: Use a *nonlinear* scheme
- Combine a low-order (guaranteed to be monotonic) with a high-order (more accurate) scheme in a nonlinear fashion



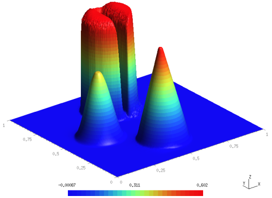
exact



low-order

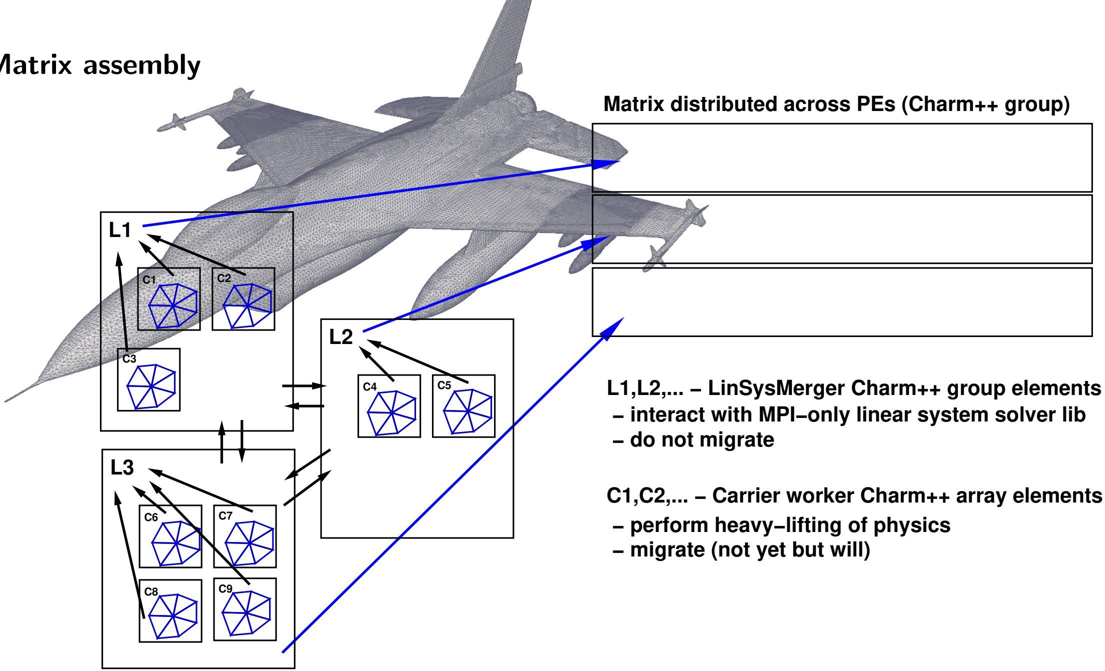


high-order



FCT

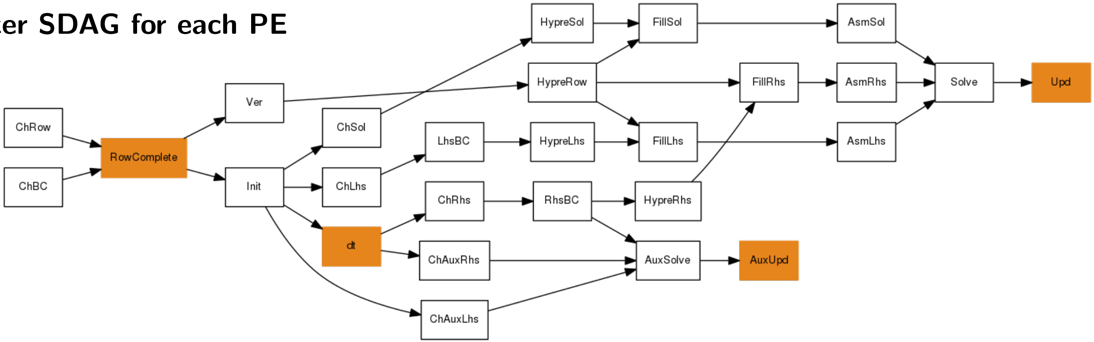
Matrix assembly



L1,L2,... – LinSysMerger Charm++ group elements
- **interact with MPI–only linear system solver lib**
- **do not migrate**

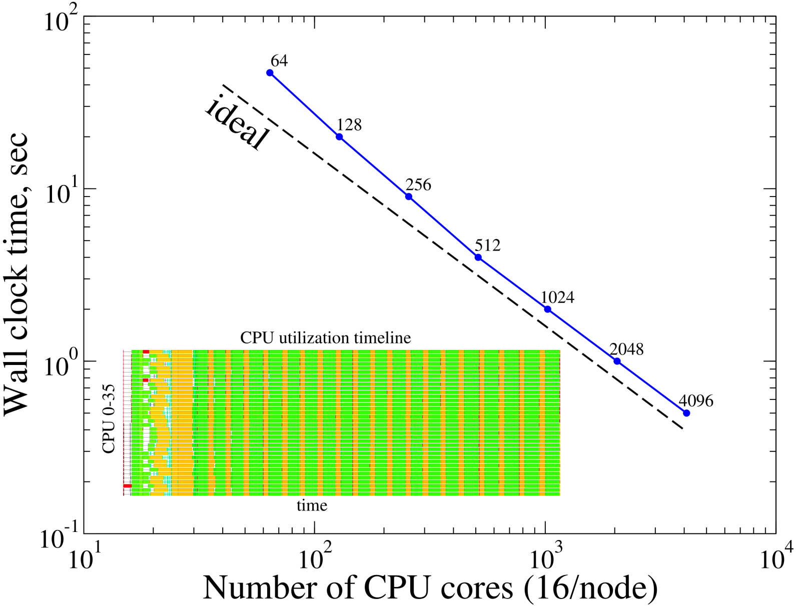
C1,C2,... – Carrier worker Charm++ array elements
- **perform heavy–lifting of physics**
- **migrate (not yet but will)**

Inciter SDAG for each PE

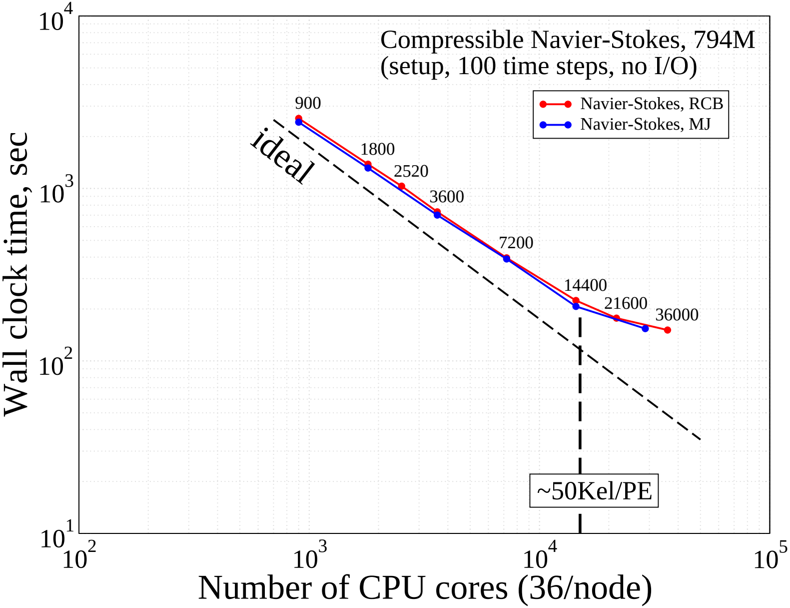


ChRow – chares contribute their global row IDs
ChBC – chares contribute their BC node IDs
RowComplete – all groups have finished their row IDs
Init – chares initialize
dt – chares compute their next Δt
Aux – Low order solution
Solve – Call hypre to solve linear system
Asm* – Assemble RHS/LHS/UNK
Hypre* – Convert RHS/LHS/UNK to hypre data structure

src/LinSys/linsysmerger.ci



Wall clock time, sec
Number of CPU cores (16/node)
ideal
64
128
256
512
1024
2048
4096
CPU utilization timeline
CPU 0-35
time



Compressible Navier-Stokes, 794M
(setup, 100 time steps, no I/O)
Navier-Stokes, RCB
Navier-Stokes, MJ
ideal
900
1800
2520
3600
7200
14400
21600
36000
~50Kel/PE
Wall clock time, sec
Number of CPU cores (36/node)

Quinoa::Inciter future plan

- **Now:** Distributed-memory-parallel asynchronous AMR
- **Next:** Explore scalability with large load-imbalances (migration)
- **Future:**
  - Asynchronous I/O
  - Explore various threading and SIMD abstractions
  - Explore CERN's ROOT framework for data storage, statistical analysis, and visualization
  - Fault tolerance

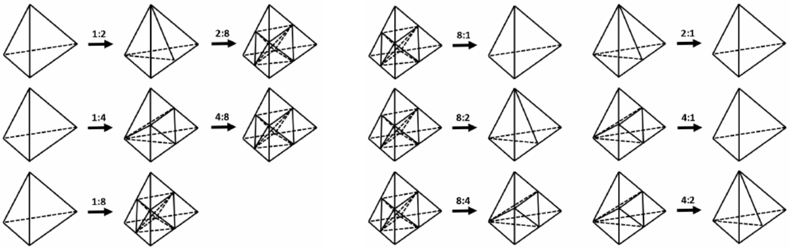


Figure 2: Allowable refinement (left) and derefinement (right) patterns

Waltz, Int. J. Numer. Meth. Fluids, 2004.

Acknowledgments

TPLs: Charm++, Parsing Expression Grammar Template Library, C++ Template Unit Test Framework, Boost, Cartesian product, PStreams, HDF5, NetCDF, Trilinos: SEACAS, Zoltan2, Hypre, RNGSSE2, TestU01, PugiXML, BLAS, LAPACK, Adaptive Entropy Coding library, libc++, libstdc++, MUSL libc, OpenMPI, Intel Math Kernel Library, H5Part, Random123

Compilers: Clang, GCC, Intel

Tools: Git, CMake, Doxygen, Ninja, Gold, Gcov, Lcov, NumDiff