

LA-UR-04-2937

*Approved for public release;  
distribution is unlimited.*

*Title:* PROGRESS REPORT FOR THE CAPSAICIN PROJECT

*Author(s):* K. Thompson

*Submitted to:* Workshop V on Parallel Transport  
April 30 - May 1, 2004  
College Station, Texas



Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the University of California for the U.S. Department of Energy under contract W-7405-ENG-36. By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

COMPUTER & COMPUTATIONAL  
SCIENCES



# Progress Report for the Capsaicin Project (U)

Kelly Thompson

Workshop V on Parallel Transport

*April 30 - May 1, 2004*

Computer and Computational Sciences Division  
Transport Methods Group (CCS-4)  
Voice: 505-665-3929 Fax: 505-665-5538  
kgt@lanl.gov <http://www.ccs.lanl.gov>



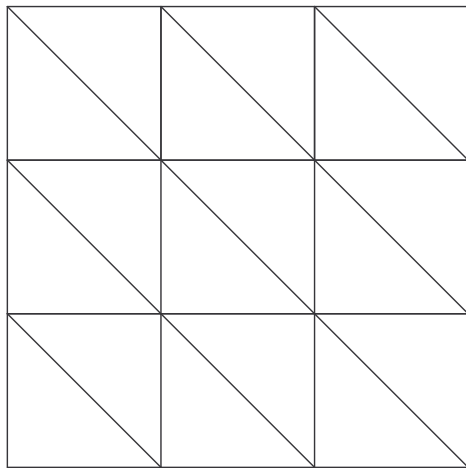


# What I'm going to tell you...

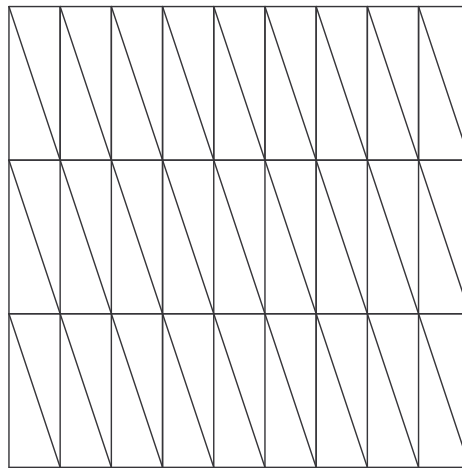
- n Focus is moving away from ROCOTILLO and toward SERRANO.
  - u Milestone driven development.
  - u What are these codes? What do they do?
- n SQI
  - u What is the Capsaicin Team doing? Why?
  - u What else is there? How we decide what to do?
- n Preliminary results
  - u MMS & example problem.
- n Capsaicin Roadmap
  - u What are our goals?
  - u How do we do incremental component/application development?

# Last time our focus was on ROCOTILLO

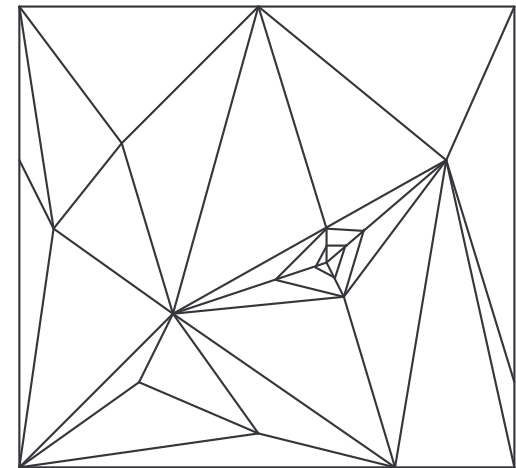
- n At Workshop IV:
  - u Kent Budge reported on ROCOTILLO.
  - u Benchmark a code that solves the streaming plus collision operator.
  - u Triangular meshes, domain decomposition.



Square



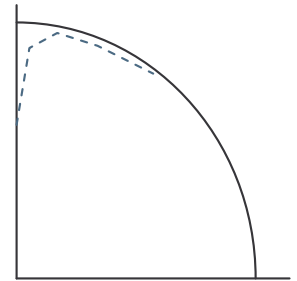
High Aspect



Random

# Today our focus is on SERRANO

- n SERRANO has the following features:
  - u Solves 1<sup>st</sup> order form of the time dependent radiative transfer equation.
  - u Discrete ordinates angular discretization.
  - u LLD spatial discretization (Morel)
    - F 2<sup>nd</sup> order accurate, good diffusion limit, no flux dip
  - u Track ion, electron and radiation temperatures (but no electron conduction yet).
  - u Use analytic and tabular opacity models.
  - u Thompson scattering, linearized Planck emission.
  - u Reflective, source, vacuum boundaries.
  - u Parallel sweep and parallel block-Jacobi algorithms.



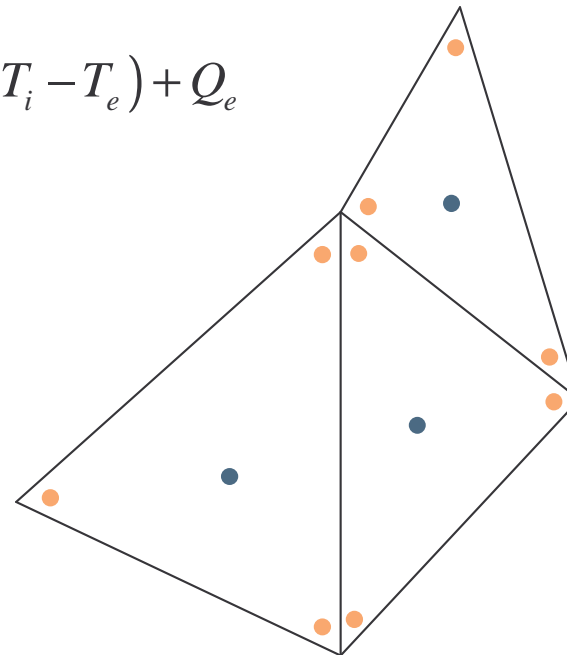
# SERANO solves the 3T problem

- n 3T radiative transfer equations.
- n Discretized to be implicit in time, multi-group, discrete ordinates, and Morel's LLD for RZ triangles.

$$\frac{1}{c} \frac{\partial I}{\partial t} + \bar{\Omega} \cdot \bar{\nabla} I + \rho \kappa_a I(\bar{x}, \bar{\Omega}, \nu, t) = \rho \kappa_s I + \rho \kappa_a \beta(T_e) + Q_r$$

$$\rho C_{v_e} \frac{\partial T_e}{\partial t} = \bar{\nabla} \cdot k_e \bar{\nabla} T_e - \rho \kappa_a \beta(T_e) + \rho \kappa_a I + \tau_{ie} (T_i - T_e) + Q_e$$

$$\rho C_{v_i} \frac{\partial T_i}{\partial t} = \underbrace{\bar{\nabla} \cdot k_i \bar{\nabla} T_i}_{\approx 0} + \tau_{ie} (T_e - T_i) + Q_i$$



- Solution values
- Material Properties



# Capsaicin Software Quality

## SQ[AEIOU] – What we are doing right now:

- n Use documentation to take control of project
  - u Vision, scope, elicitation, requirements, design specification, implementation plan, release note.
  - u Physics manual, users manual, developer notes, project process documents.
- n Reviews
  - u Design and code reviews, pair programming.
  - u Refactor only when required.
- n From project initiation,
  - u Design is parallel, object-oriented, levelized.
  - u Automatic documentation.



# More SQE buzz-words...

- n Testing
  - u Design-by-Contract
  - u Integrated (physics) and unit (software) testing.
  - u Regression (delta over time) testing and application (code-to-code, gold standard, analytics) testing.
- n Revision Control
  - u Source is under CVS control
  - u Documents under change management (SF)  
We use an iterative staged delivery process.
  - u Bug tracking. Fixes tied to specific release.
- n SQE should empower a project to learn from mistakes, make educated decisions and save time.

# Code Metrics and Levelized Design

## n Code Metrics

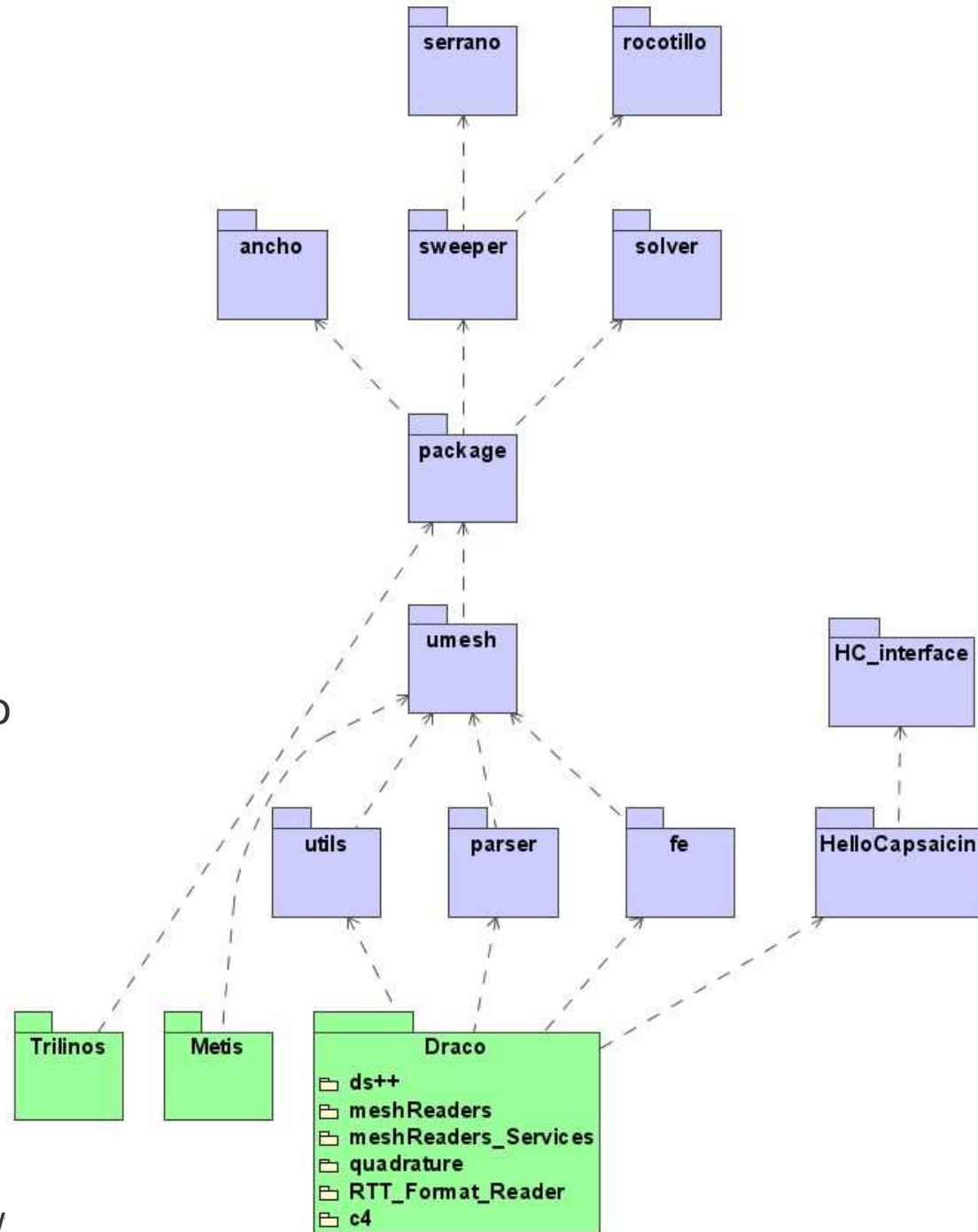
- u 20000 lines of code
- u 6600 lines of test code (++)
- u 1000 contract specifications
- u 20000 lines of comments

## n Instrumentation

- u Purify, Insure++
- u STLport
- u Code coverage reports tied to testing.

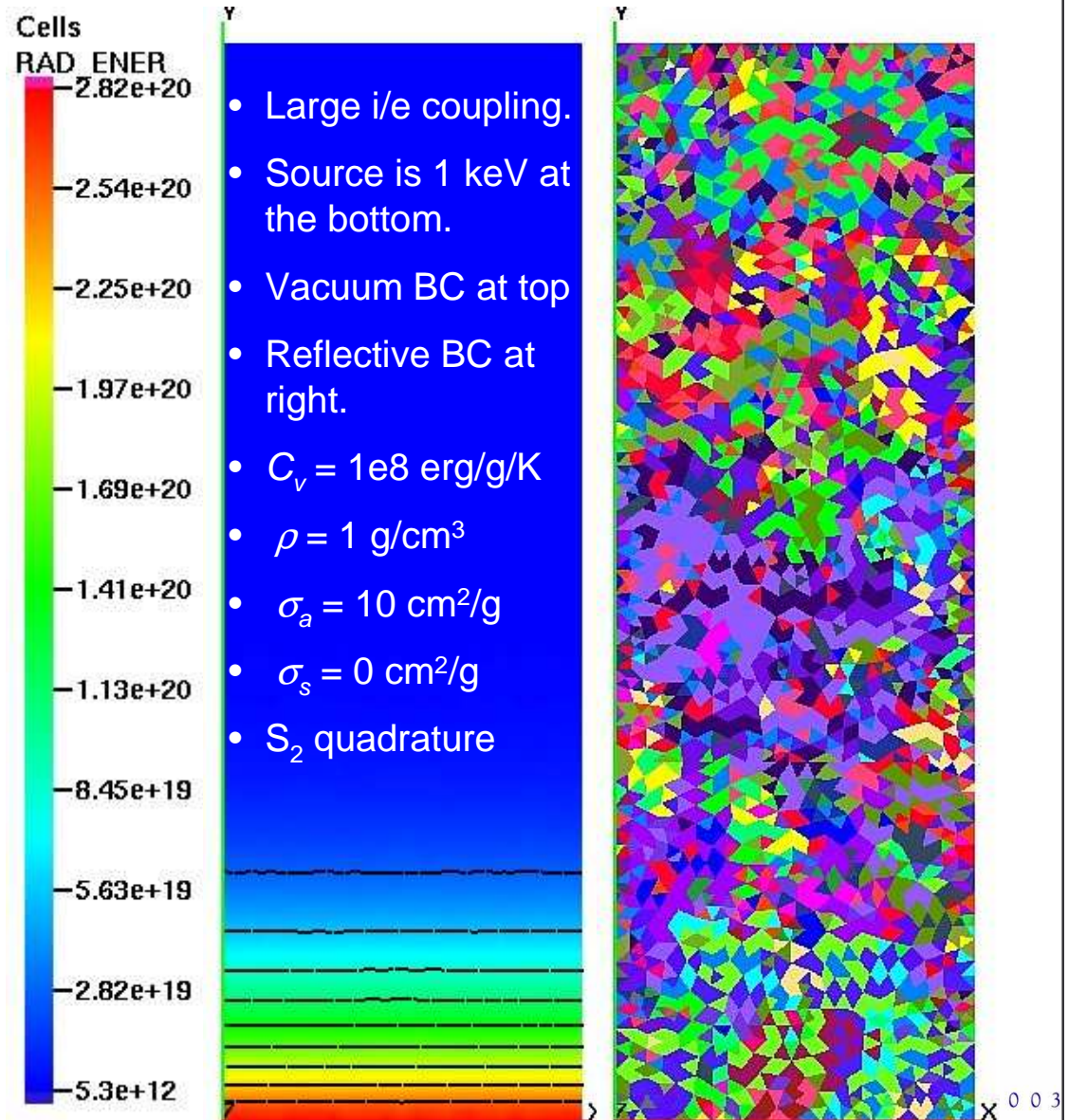
## n 3<sup>rd</sup> party vendors

- u MPI, mpich, LA-MPI communication models.
- u Draco, Trilinos, Metis, LAPACK, LANL materials libraries.



# Heat flow demonstration problem

- Demonstration problem only.
- Not a verification problem.
- Source  $T = 1$  keV
- Reflective BC on L/R.
- Unstructured mesh with random cell-set groups.
- Use Warsa's python mesh generator.
- Ready to run analytic Marshak (w/o DSA) – but lets not get ahead of ourselves – incremental feature testing.



# Manufactured Solutions

n MMS is to dream up a solution  $I$ , evaluate the corresponding source  $S$  analytically, then feed  $S$  to the sweeper to see if we recover a good solution of the original manufactured solution  $I$ .

n Should be used when it is easy to obtain  $S$  from  $I$  but hard to go from  $I$  to  $S$ .

n For example, let the solution be

$$I(r, z) = e^{z-r^2}$$

n So that the driving source must be

$$Q - \sigma_a I = (\xi - 2\mu r) e^{z-r^2}$$

n Now run the code with the provided  $Q$  to see if it can compute  $I$ .

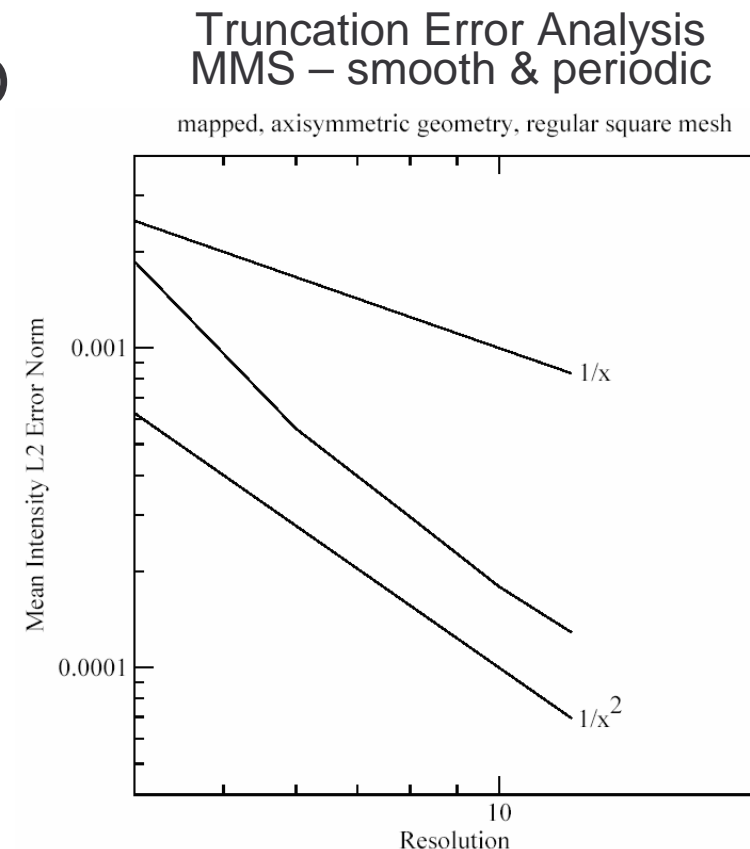
n ROCOTILLO obtains the correct solution but appears 1<sup>st</sup> order accurate. Why?

# MMS & Truncation Error Analysis

- n Choice of MS is unfortunate. It is not a smooth solution. Try a periodic solution for this measure.

$$I(r, z) = \cos(2\pi r) \cos(2\pi z) + \mu [1 - \cos(2\pi r)] \cos(2\pi z)$$

- n Using manufactured solutions we have demonstrated that SERRANO is 2<sup>nd</sup> order accurate in space (XY and RZ) and angle.
- n Be careful when using MMS!





# Code Roadmap

- n Now – Oct 1, 2004
  - u **Verification**, release and report.
  - u DSA implementation.
- n FY05
  - u ASC Milestone.
  - u Stand alone diffusion solver.
  - u Better time step controller.
  - u Hybrid (triangles plus quadrilaterals) mesh support?
- n Long term
  - u Electron conduction model, Compton scattering model.
  - u 3D tetrahedral, adaptive in angle
  - u Can we use subzone mapping to treat polygon meshes and other special mesh feature treatments.



# Research Roadmap

- n Continue to examine properties of lumped LD discretizations.
  - u Are lumped discretizations needed for time dependent radiative transfer?
  - u What are the real (dis)advantages of lumped methods? Are there alternatives?
- n Parallel block-Jacobi solutions.
  - u We need to understand why this method breaks down for small cells as  $N_p$  becomes large.
- n Can we treat all meshes with triangles?
  - u Conformal sub-zone meshes.

# Results of LD Lumping Study

	Tetrahedral Mesh				Hexahedral Mesh			
	Orthogonal		Random		Orthogonal		Random	
	1D	3D	1D	3D	1D	3D	1D	3D
Unlumped	2	2	2	2	2	2	2	2
Mass-lumped	1	2	1	2	2	2	2*	2
Fully-lumped	1	2	1	2	2	2	0	2

\* not confirmed.



# What I just told you (in case you were sleeping)

- n Focus is moving away from ROCOTILLO and toward SERRANO.
  - u Milestone driven development.
  - u What are these codes? What do they do?
- n SQI
  - u What is the Capsaicin Team doing? Why?
  - u What else is there? How we decide what to do?
- n Preliminary results
  - u MMS & example problem.
- n Capsaicin Roadmap