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Recommended Citation
Reynolds, Daniel R.; Harkness, Robert; So, Geoffrey; and Norman, Michael L., "Block preconditioning of stiff implicit models for radiative ionization in the early universe" (2012). Mathematics Research. 5.
https://scholar.smu.edu/hum_sci_mathematics_research/5

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Block preconditioning of stiff implicit models for radiative ionization in the early universe

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SIAM Parallel Processing for Scientific Computing
February 17, 2012
Outline

1. Science
   - Reionization
   - Model

2. Solution Approach
   - Framework
   - Implicit Subsystem
   - Solvers

3. Numerical Results
   - Verification and Scaling
   - Reionization Simulations

4. Conclusion
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Cosmic Reionization – The Origins of the Universe

- Dark Energy
- Accelerated Expansion
- Development of Galaxies, Planets, etc.
- Afterglow Light Pattern
  380,000 yrs.
- Dark Ages
- Inflation
- Quantum Fluctuations
- 1st Stars
  about 400 million yrs.

Big Bang Expansion
13.7 billion years
Cosmic Reionization – The Origins of the Universe

- What were the dominant physical processes governing star and cluster formation in the early universe?

- Can modern physics models predict the processes of formation and cosmological reionization?

- Optical telescopes can only look back to the Epoch of Reionization, due to optically-thick neutral gases following the Big Bang.

- New WMAP telescope (infra-red) enables further studies, allowing first-ever validation/repudiation of reionization theories.
We study these questions using the *Enzo* code, modeling gravity, gas dynamics, chemical ionization and radiation transport in an expanding universe:

\[
\nabla^2 \phi = \frac{4\pi G}{a} (\rho_b + \rho_{dm} - \rho_0),
\]

\[
\partial_t \rho_b + \frac{1}{a} \mathbf{v}_b \cdot \nabla \rho_b = -\frac{1}{a} \rho_b \nabla \cdot \mathbf{v}_b,
\]

\[
\partial_t \mathbf{v}_b + \frac{1}{a} (\mathbf{v}_b \cdot \nabla) \mathbf{v}_b = -\frac{\dot{a}}{a} \mathbf{v}_b - \frac{1}{a \rho_b} \nabla p - \frac{1}{a} \nabla \phi,
\]

\[
\partial_t e + \frac{1}{a} \mathbf{v}_b \cdot \nabla e = -\frac{2\dot{a}}{a} e - \frac{1}{a \rho_b} \nabla \cdot (p \mathbf{v}_b) - \frac{1}{a} \mathbf{v}_b \cdot \nabla \phi + G - \Lambda,
\]

\[
\partial_t n_i + \frac{1}{a} \nabla \cdot (n_i \mathbf{v}_b) = -n_i \Gamma_i^{ph} + \alpha_{i,j} n_e n_j, \quad i, j = 1, \ldots, N_{chem},
\]

\[
\partial_t E + \frac{1}{a} \nabla \cdot (E \mathbf{v}_b) = \nabla \cdot (D \nabla E) - \frac{\dot{a}}{a} E - c\kappa E + 4\pi \eta,
\]

Along with a Lagrangian model for dark matter particle dynamics.

Here, \(\Delta t_{n_i} < \Delta t_E \ll \Delta t_{\text{hydro}}\).

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Simulation Framework

We approximate solutions with a method of lines operator-split approach:

- Domain $\Omega = [0, L]^3$ ($L \gtrsim 10$ comoving Mpc, or $\gtrsim 10^{20}$ km) discretized using finite volumes via uniform grids or block-structured AMR\textsuperscript{1}.

- Long-time evolution ($z$ from $100 \rightarrow 5$), approximately 2 Gyr.

- Explicit hydrodynamic evolution and passive advection via PPM\textsuperscript{1}.

- Advect dark matter particles via Particle-Mesh method\textsuperscript{2}.

- FFT or MG-based solve for the gravitational potential $\phi$.

- Implicit evolution of stiff radiation & chemistry with gas energy feedback.

This talk focuses on the stiff subsystem coupling the grey radiation energy density $E$, primordial chemical abundances $n_i$, and gas energy correction $e_c$:

$$\partial_t e_c = -2\frac{\dot{a}}{a} e_c + G - \Lambda,$$
$$\partial_t n_i = -n_i \Gamma_{i}^{ph} + \alpha_{i,j} n_e n_j, \quad i, j = \{\text{HI, HeI, HeII}\},$$
$$\partial_t E = \nabla \cdot (D \nabla E) - \frac{\dot{a}}{a} E - c\kappa E + 4\pi\eta.$$

- $G(n_i, E)$ and $\Lambda(e, n_i)$ provide photo-heating and thermal cooling.
- $\Gamma_{i}^{ph}(E)$ is photo-ionization, and $\alpha_{i,j}(e, n_i)$ are reaction rates.
- $\kappa(n_i)$ is the opacity, $D(\kappa, E)$ a flux limiter, and $\eta$ an emissivity source.

Due to these strong interconnections, we solve this as a coupled implicit system to help ensure stability/accuracy.
Implicit Time Discretization

We consider a $\theta$-scheme for implicit integration of the RT subsystem:

\[ e^n_c + \theta \Delta t \mathcal{L}_e (e^n_c, n^n_i, E^n) = g^{n-1}_e, \]
\[ n^n_i + \theta \Delta t \mathcal{L}_n (e^n_c, n^n_i, E^n) = g^{n-1}_{n_i}, \]
\[ E^n + \theta \Delta t [\mathcal{D}_E (E^n) + \mathcal{L}_E (e^n_c, n^n_i, E^n)] = g^{n-1}_E. \]

where $g^{n-1}_*$ provide data from the previous time step.

Denoting our unknowns as $U = [e_c, n_i, E]^T$, we define a nonlinear residual, $f(U)$, over the time step $t^{n-1} \rightarrow t^n$ as

\[ f(U) = U + \theta \Delta t \begin{bmatrix} \mathcal{L}_e \\ \mathcal{L}_n \\ \mathcal{D}_E + \mathcal{L}_E \end{bmatrix} - g^{n-1}. \]
Nonlinear Solver: $f(U) = 0$

We solve $f(U) = 0$ for $U^n$ using a *globalized inexact Newton method*:

$$J(U_k) S_k = -f(U_k), \quad U_{k+1} = U_k + \lambda_k S_k, \quad k = 0, 1, \ldots$$

**Details:**

- Iterate until $\|f(U_k)\| < \varepsilon$, $0 < \varepsilon \ll 1$.
- $S_k$ is solved inexact, $\|J_k S_k + f_k\| < \delta$, $0 < \delta \ll 1$.
- $\lambda_k \in (0, 1]$ is the *line search* parameter.
- $\|\cdot\|$ is a $L$-2 norm weighted by relative magnitudes of $U^{n-1}$.
- Rapid, resolution-independent convergence for many PDE systems.
- Efficiency rests on a fast/scalable solver for the linear Newton systems.

We note that these Jacobian matrices have the form

$$J(U) = I + \theta \Delta t \begin{bmatrix} \partial_e \mathcal{L}_e & \partial_n \mathcal{L}_e & \partial_E \mathcal{L}_e \\ \partial_e \mathcal{L}_n & \partial_n \mathcal{L}_n & \partial_E \mathcal{L}_n \\ \partial_e \mathcal{L}_E & \partial_n \mathcal{L}_E & \partial_E(\mathcal{L}_E + \mathcal{D}_E) \end{bmatrix}.$$

[see Dembo et al., 1982; Brown & Saad, 1990; Allgower et al., 1986; Weiser et al., 2005]
Schur-Krylov-MG Linear Solver: \( J_s = -f \)

Combining the spatially “local” variables \( s_M = [s_e, s_n] \), we rewrite

\[
Js = -f \iff \begin{bmatrix} M & U \\ L & D \end{bmatrix} \begin{bmatrix} s_M \\ s_E \end{bmatrix} = -\begin{bmatrix} f_M \\ f_E \end{bmatrix}.
\]

\( M^{-1} \) is simple to compute (block-diagonal), so we use a Schur complement formulation to solve for \( s \),

\[
M s_M + U s_E = -f_M \iff s_M = -M^{-1}(f_M + U s_E),
\]
\[
\Rightarrow (D - L M^{-1} U) s_E = L M^{-1} f_M - f_E.
\]

Details:
- \( (D - L M^{-1} U) s_E = L M^{-1} f_M - f_E \) solved with a CG iteration.
- CG preconditioned using geometric multigrid [HYPRE-PFMG].
- \( s_M \) is then easily computed from \( s_E \).
**MPI+OpenMP Hybrid Parallelization**

- Threading needed to minimize memory footprint for Enzo data structures.
- Groups of cores are clustered into a single MPI task.
- Physics modules use threading within each MPI task.
- Newton solve needs only neighbor communication and infrequent MPI_Allreduce calls.
- Schur complement formulation is inherently processor-local.
- HYPRE allows hybrid parallelism; performance is a work in progress (version 2.7.0b at right).
- Parallel I/O uses HDF5.

The graph shows the weak scaling of ENZO RHD with 3 MPI tasks per node from June 2011.
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**Verification Tests and Weak Scaling**

**NW**: isothermal, static I-front convergence.

**NE**: hydrodynamic I-front convergence.

**SW**: cosmological, static I-front convergence.

**SE**: weak scaling ($N_{src} \propto N_{CPU}$) on Kraken [NICS].

Reionization $(1024^3 \text{ grid, 4096 cores, 5.6 Mpc box})$

\[ \rho \]
\[ E \]
\[ x_{\text{HI}} \]

- $z = 15$
- $z = 11$
- $z = 8$
- $z = 6$
Multiscale Issues – Space and Time

Many cosmological problems require spatial adaptivity:

- At high redshift, \( \rho \) is diffuse and fills the whole domain.
- As structures form the majority of the volume empties.
- AMR can reduce memory requirements at low \( z \) by orders of magnitude.

Coupled \( \Delta t \) selection is difficult:

- At star creation, emissivities jump by orders of magnitude.
- Enclosing cells ionize rapidly, with \( x_{\text{HI}} \) quickly decreasing by \( O(10^5) \).
- Naïve integrators may overshoot, resulting in negative densities.
- Production runs create \( O(10^8) \) stars, so this is not an isolated event.
- Hence, current production runs (\( \sim 47k \) cores) decouple chemistry from the radiation system, allowing subcycling to maintain physicality.
  - This splitting decreases accuracy, but increases robustness.
  - \( \Delta t \) must be reduced to produce accurate physics (e.g. \( r_I \) speed).
Current Work

Extending solvers to AMR grids:

- Implicit AMR presents new challenges:
  - matrix stencils at coarse-fine interfaces,
  - proper nesting of refined regions,
  - global time step selection balancing cell size contributions,
  - multigrid + AMR is nontrivial.

- FAC\(^1\) gravity solver already completed (James Bordner).

- FLD extension complete; in testing/optimization stages now.

New time integration methods:

- Split couplings may be improved with ARK\(^2\) or SDC\(^3\) methods.

- Predictive $\Delta t$ control based on star formation.

- Chemistry model may be adapted between dynamic and steady-state solvers based on local dynamics.

\[^1\]McCormick, 1989; \(^2\)Cooper & Sayfy, 1983; \(^3\)Ascher et al., 1997; Minion, 2003; Hagstrom & Zhou, 2006\]
Acknowledgements

We gratefully acknowledge support by:

- US National Science Foundation – AAG and OCI programs
- US Department of Energy – INCITE program
- NCSA Blue Waters program

Collaborator contributions:

- UC San Diego – Michael Norman, James Bordner, Geoffrey So
- SDSC – Robert Harkness, Michael Norman, Richard Wagner
- LLNL – John Hayes (B-Division)
- Northwestern – Pascal Paschos

Open-source software:

- Enzo – http://enzo.googlecode.com
- HDF5 – http://www.hdfgroup.org
Reionization Visualization (SC 2011)