Randomized Orthogonal Projection Methods for Krylov solvers

Edouard Timsit[1], Laura Grigori[1], Oleg Balabanov[2]

May 15, 2023

[1]Sorbonne Université, Inria, CNRS, Université de Paris, Laboratoire Jacques-Louis Lions, Paris, France

[2]Part of this work was conducted while the author was at Sorbonne Université, Inria, CNRS, Université de Paris, Laboratoire Jacques-Louis Lions, Paris, France

Introduction to Krylov solvers

Krylov solvers ? A mathematical setting describing several iterative methods.

Define linear system of equations with first guess $x_0 \in \mathbb{R}^n$

$$Ax = b, \quad A \in \mathbb{R}^{n\times n}, \quad b \in \mathbb{R}^n$$

Seek solution in the Krylov subspace, $r_0 = b - Ax_0$

$$\mathcal{K}_k(A, r_0) = x_0 + \mathrm{Span}\langle r_0, Ar_0, \cdots, A^{k-1}r_0\rangle$$

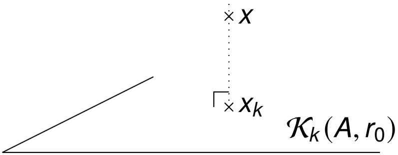
Designing a Krylov solver

For all $k \leq n$, find $x_k \in \mathcal{K}_k(A, r_0)$ that **minimizes some measure of the error $x - x_k$**

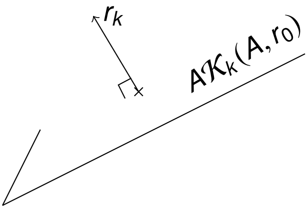
Example : Choose $x_k = \arg\min_{y \in \mathcal{K}_k(A, r_0)} \|x - y\|_2$

Reformulate with the residual $r_k = b - Ax_k$:

$$x_k = \arg\min_{y \in \mathcal{K}_k(A, r_0)} \|x - y\|_2 \iff r_k \perp A\mathcal{K}_k(A, r_0)$$



(a) Some Krylov design



(b) Equivalent formulation

Mathematical formulation

We've designed a Krylov solver. An iterative method producing $(x_k)_k$ s.t :

1. $\forall k,\ x_k \in \mathcal{K}_k(A, r_0)$ *(subspace condition)*
2. $\forall k,\ r_k \perp \mathcal{L}_k$, with $\mathcal{L}_k$ some k-dimensional vector subspace *(Petrov-Galerkin condition)*

Examples [6] :

- CG : $r_k \perp \mathcal{K}_k(A, r_0) \iff x_k = \arg\min_{y \in \mathcal{K}_k(A,r_0)} \|x - y\|_A$
- GMRES :
  $r_k \perp A\mathcal{K}_k(A, r_0) \iff x_k = \arg\min_{y \in \mathcal{K}_k(A,r_0)} \|b - Ay\|_2$

A problem arises

How to enforce the Petrov-Galerkin condition ?

$$\mathcal{P}_{\mathcal{L}_k}(b - Ax_k) = 0 \iff (\mathcal{P}_{\mathcal{L}_k}A)x_k = (\mathcal{P}_{\mathcal{L}_k}b) \qquad (x_k \in \mathcal{K}_k(A, r_0))$$

Usually requires access to bases of $\mathcal{L}_k$ and of $\mathcal{K}_k(A, r_0)$. For numerical stability, these bases should be well conditioned. Not the case of $\{r_0, Ar_0, \cdots A^{k-1}r_0\}$!

$\implies$ Proceed with a subsequent orthonormalization process of these bases.

Dilemma : often the most expensive part of the solver (typical asymptotic cost is $\mathcal{O}(nk^2)$ flops)

Introduction to randomization

Randomization ? A dimension reduction technique that approximates geometry of a vector-subspace $\mathcal{V}_k \subset \mathbb{R}^n$, $k \ll n$.

We say that a linear mapping $\Omega : \mathbb{R}^n \to \mathbb{R}^\ell$ is an ϵ-embedding of $\mathcal{V}_k$ if and only if

$$\forall x \in \mathcal{V}_k, \quad (1-\epsilon)\|x\|_2^2 \le \|\Omega x\|_2^2 \le (1+\epsilon)\|x\|_2^2 \qquad (1)$$

see [8]. Due to parallelogram identity, eq. (1) is equivalent to

$$\forall x, y \in \mathcal{V}_k, \ |\langle \Omega x, \Omega y\rangle - \langle x, y\rangle| \le \epsilon \|x\|_2 \|y\|_2$$

Typical $\epsilon = \frac{1}{2}$. Designed to preserve orders of magnitude, not to be a fine approximation.

An analogy with projections (1)

(a) Enough to guess geometry...

(b) ...but can be misleading !

Figure: Good and bad projections

An analogy with projections (2)

Figure: A set of high-dimensional vectors projected in $\mathbb{R}^3$ (*diadema urchin*)

Oblivious subspace embeddings

Oblivious subspace embedding with parameters ϵ, k, δ : a linear mapping[3] $\Omega : \mathbb{R}^n \to \mathbb{R}^\ell$ such that, for any k-dimensional subspace $\mathcal{V}_k$, it is an ϵ-embedding of $\mathcal{V}_k$ with probability at least $1 - \delta$ (see [8]).

Examples :

- Gaussian OSE : Independent $\Omega_{i,j} \sim \mathcal{N}(0, \sqrt{\ell}^{-1}), \quad 1 \leq j \leq \ell$.
  Dense matrix.
- SRHT OSE : Independent ℓ rows sampling of HD where $H \in \mathbb{R}^{n \times n}$ is Hadamard transform and D is random cheap rotation.
  Fast transform, but not suited for distributed computing [9]

ℓ : the sampling size. The more successful and fine we want Ω, the greater the sampling size. Typical $\ell = 5k$.

---

[3] The theory is simplified here

Some new notions

Let $\Omega : \mathbb{R}^n \to \mathbb{R}^\ell$ an ϵ-embedding for vector subspace $\mathcal{V}_k$. Let $\mathcal{V}_p \subset \mathcal{V}_k$ a vector subspace.

- We say that $v_1, \cdots, v_p \in \mathcal{V}_p$ are a sketch orthonormal basis of $\mathcal{V}_p$ if and only if they are a basis of $\mathcal{V}_p$ and verify

$$\forall i,j \in \{1, \cdots p\}, \quad \langle \Omega v_i, \Omega v_j \rangle = \delta_{i,j} \qquad \left(\mathrm{Cond}(V_p) \leq \sqrt{\frac{1+\epsilon}{1-\epsilon}}\right)$$

- We say that $z \perp^{\Omega} \mathcal{V}_p$ if and only if

$$\forall x \in \mathcal{V}_p, \quad \langle \Omega z, \Omega x \rangle = 0$$

- We define the sketch orthogonal projector from $\mathcal{V}_k$ onto $\mathcal{V}_p$ as

$$\mathcal{P}^{\Omega}_{\mathcal{V}_p} : \begin{cases} \mathcal{V}_k & \to & \mathcal{V}_p \\ x & \mapsto & \arg\min_{y \in \mathcal{V}_p} \|\Omega(x-y)\|_2^2 \end{cases}$$

Problem identified

Replace the orthogonalization step of Krylov solvers by sketch-orthogonalization step ?

What has been done :

- Randomized Gram-Schmidt [2] and block version [1] : Half the flops of modified Gram-Schmidt (MGS), with similar stability.
- Applied to GMRES [2], same convergence rate, stable.
- Applied to eigenvalue solvers [5]

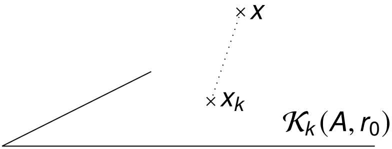
The case $r_k \perp^{\Omega} A\mathcal{K}_k(A, r_0)$ is now well documented. What about $r_k \perp^{\Omega} \mathcal{K}_k(A, r_0)$?

Considered in [3, 4], but still no error minimizing characterization.

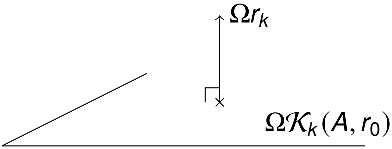
ROPMs

Randomized Orthogonal Projection Method over the Krylov subspace (ROPM) : an iterative algorithm producing $(x_k)_k$ s.t :

1. $\forall k, x_k \in \mathcal{K}_k(A, r_0)$ *(subspace condition)*
2. $\forall k, r_k \perp^{\Omega} \mathcal{K}_k(A, r_0)$ *(sketched Petrov-Galerkin condition)*



(a) In $\mathbb{R}^n$...



(b) ...embedded in $\mathbb{R}^\ell$

RFOM

The following algorithm is an ROPM.

Input: Matrix $A \in \mathbb{R}^{n \times n}$, vector $b \in \mathbb{R}^n$, ϵ-embedding $\Omega \in \mathbb{R}^{\ell \times n}$ of $\mathcal{K}_{k_{\max}}$, $k_{\max} < \ell \ll n$, first guess x_0

Output: Approximation $x_k \in \mathcal{K}_k(A, r_0)$ of solution to $Ax = b$.

```
r_0 ← b − A x_0
Compute Ω r_0
v_1 ← ||Ω r_0||^{-1} r_0
Compute/deduce Ω v_1
while k ≤ k_max and ||Ω r_k|| > η do
    w ← A v_k
    Compute Ω w
    (h_{i,k})_{1≤i≤k} ← (Ω V_k)^t Ω w where V_k is the matrix formed by
      v_1, ··· v_k
    w ← w − V_k (h_{i,k})_{1≤i≤k}
    Compute/deduce ||Ω w||
    h_{k+1,k} ← ||Ω w||
    w ← h_{k+1,k}^{-1} w
    v_{k+1} ← w
    Compute/deduce Ω v_{k+1}
    x_k ← x_0 + H_k^{-1} (Ω V_k)^t Ω r_0, where H_k = (h_{i,j})_{1≤i≤k, 1≤j≤k}
    k ← k + 1
return x_k
```

Algorithm 0: RFOM, a.k.a Randomized Arnoldi

Is the sketched Petrov-Galerkin condition met?

This algorithm builds sketch orthonormal vectors $v_1, v_2 \cdots$ s.t:

$$\forall k, \quad h_{k+1,k} v_{k+1} = A v_k - \langle \Omega A v_k, \Omega v_1 \rangle v_1 - \cdots \langle \Omega A v_k, \Omega v_k \rangle$$

We get the randomized Arnoldi relation :

$$\forall k, \; A V_k = V_{k+1} H_{k+1,k}, \quad (\Omega V_k)^t \Omega V_k = I_k, \quad H_{k+1,k} = (h_{i,j})_{\substack{1 \leq i \leq k+1 \\ 1 \leq j \leq k}}$$

Using the sketch orthogonality, we get $H_k = (\Omega V_k)^t \Omega A V_k$. Finally,

$$r_k \perp^{\Omega} \mathcal{K}_k(A, r_0) \iff (\Omega V_k)^t \Omega r_k = 0_k \iff x_k = x_0 + H_k^{-1} (\Omega V_k)^t \Omega r_0$$

Some testing (1)

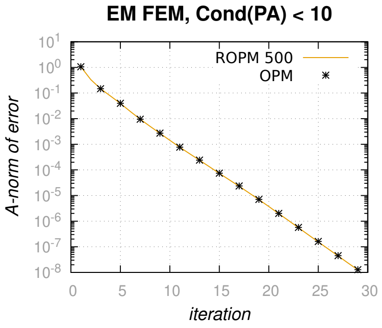
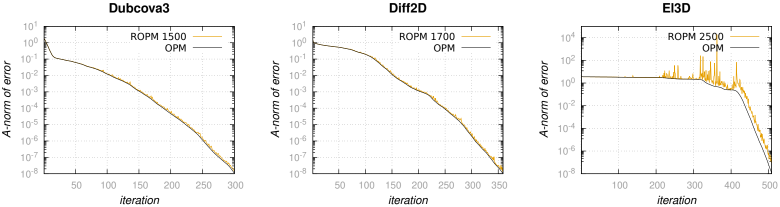


Figure: Easy problem

This is the desired behavior.

Some testing (2)



(a) Reasonably difficult system, Cond$(A) \approx 4000$

(b) Harder system, Cond$(P^{-1}A) \approx 10^5$

(c) Even harder, Cond$(P^{-1}A) \approx 10^9$

Figure: Convergence of ROPM

Similar convergence rate overall.

Apparition of spikes of the randomized error. **Are they random ?**

Straightforward bound

Using the ϵ-embedding property straightforwardly :

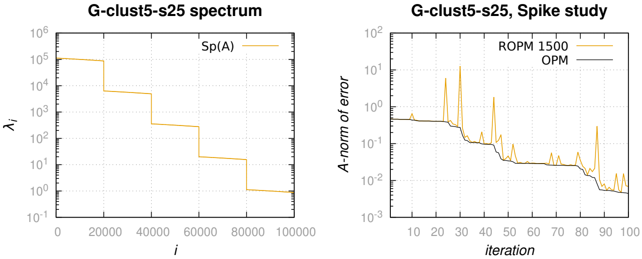
Proposition

Let $\Omega \in \mathbb{R}^{\ell \times n}$ be an ϵ-embedding of $\mathcal{K}_{k+1} + \mathrm{Span}\langle x \rangle$, with $\epsilon \leq \mathrm{cond}(A)^{-\frac{1}{2}}$. Assume that A is positive-definite. Then the estimate $x_k \in \mathcal{K}_k$ produced by ROPM and $\check{x}_k \in \mathcal{K}_k$ produced by standard OPM satisfy

$$\|x - x_k\|_A \leq \frac{1 + \epsilon\, \mathrm{cond}(A)^{\frac{1}{2}}}{1 - \epsilon\, \mathrm{cond}(A)^{\frac{1}{2}}} \|x - \check{x}_k\|_A. \tag{2}$$

Pessimistic bound. Not well-defined for ill-conditioned systems.
Doesn't describe the spikes.

Isolating the spikes



(a) Spectrum of randomly generated symmetric matrix

(b) Early convergence

Figure: Spike study

Spikes seem related to the properties of the system after all.

Our main contribution

Theorem

Assume that A is positive-definite. We have

$$\|x - x_k\|_A \leq \left(1 + \alpha_k^2 \beta_k^2\right)^{\frac{1}{2}} \|x - \check{x}_k\|_A,$$

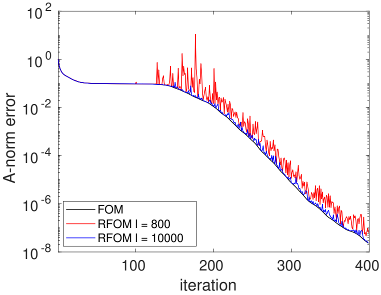
where $x_k \in \mathcal{K}_k$ and $\check{x}_k \in \mathcal{K}_k$ are the sketched and the classical Petrov-Galerkin projections, respectively, and

$$\alpha_k := \frac{\langle x - \check{x}_{k-1}, \mathcal{P}^{\Omega}_{\mathcal{K}_k} A \check{v}_k \rangle}{\langle x - \check{x}_{k-1}, \mathcal{P}_{\mathcal{K}_k} A \check{v}_k \rangle},$$

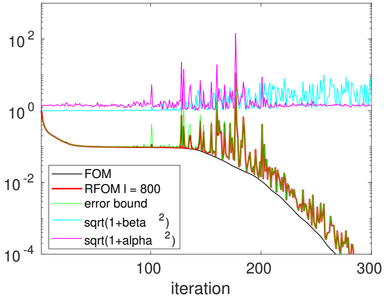
$$\beta_k := \|A^{-\frac{1}{2}} \mathcal{P}^{\Omega}_{\mathcal{K}_k} \check{v}_{k+1}\| \langle \check{v}_{k+1}, A \check{v}_k \rangle \frac{\langle \check{v}_k, \check{x}_k \rangle}{\|x - \check{x}_k\|_A},$$

and where $\check{v}_k$ is a unit vector spanning the range of $(I - \mathcal{P}_{\mathcal{K}_{k-1}})\mathcal{P}_{\mathcal{K}_k}$.

Numerical testing



(a) RFOM convergence.



(b) Effect of α_k and β_k on irregularity of RFOM.

Figure: RFOM convergence for the shifted *Si41Ge41H72* system.

Fine bound. Truthful to the sppikes.

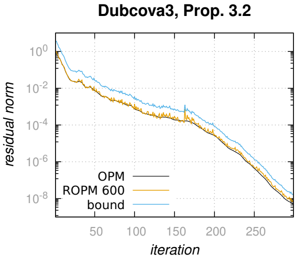
Indirect bound

Proposition

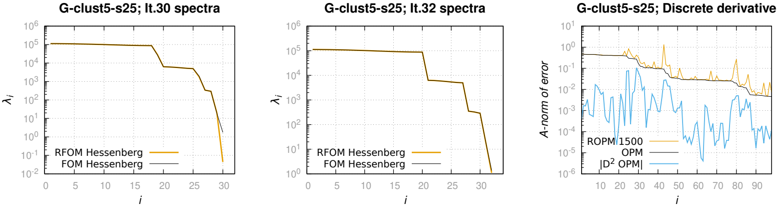
If $x_k \in \mathcal{K}_k$ satisfies the sketched Petrov-Galerkin condition, and if $\breve{x}_k$ satisfies the Petrov-Galerkin condition,

$$\|r_k\|_2 \leq \|\breve{r}_k\|_2 + \|r_0\| \left[|\breve{s}_{k,1}| + \sqrt{\frac{1+\epsilon}{1-\epsilon}} \, |s_{k,1}| \right]. \tag{4}$$

where $s_{k,1}$ (resp. $\breve{s}_{k,1}$) denote the product of $h_{k+1,k}$ and the bottom left corner of H_k^{-1} (resp ...)



Future developement



(a) Spectra at spike's iteration 30

(b) Spectra after spike iteration 32

(c) Discrete second derivative of OPM error (D^2OPM)

Figure: Spike study

Is there a synthetic bound, only featuring spectral properties of Hessenberg matrices ?

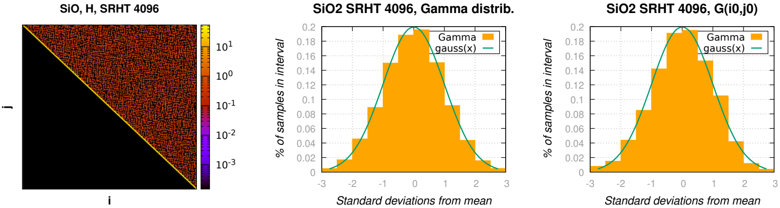
Deflation of the bad Ritz vectors ?

Short recurrences

The randomized Arnoldi relation for symmetric system A is not symmetric anymore.

$$\breve{H}_k = \breve{V}_k^t A \breve{V}_k \;\; \text{symmetric, but} \;\; (\Omega V_k)^t \Omega A V_k \neq (\Omega A V_k)^t \Omega V_k$$

Short recurrence is lost



(a) 4096 sampling size (b) Overall distribution (c) Γ_{i_0,j_0} distribution

Figure: Distribution of H_k (noise above the superdiagonal)

Noise seems Gaussian

Experimentally, Gaussian distributed noise of great magnitude above the superdiagonal.

Empirical implications : not compressible, stable by isometric transformations.

Randomization extended to CG is not trivial.

What happens if we use it anyway ?

arCG

Input: $A \in \mathbb{R}^{n\times n}$ an SPD matrix, $b \in \mathbb{R}^n$, $\eta \in \mathbb{R}^{+*}$, $k_{\max} \in \mathbb{N}^*$,
$x_0 \in \mathbb{R}^n$, Ω an ϵ-embedding of $\mathcal{K}_{k_{\max}}$
Output: x_k an estimate of the solution of $Ax = b$

$r_0 \leftarrow b - Ax_0$
$p_0 \leftarrow r_0$
Compute Ωr_0
while $\|\Omega r_k\| \geq \eta \|b\|$ ***and*** $k \leq k_{max}$ **do**
  if $k \geq 1$ **then**
    $\delta_k \leftarrow \frac{\|\Omega r_k\|^2}{\|\Omega r_{k-1}\|^2}$
    $p_k \leftarrow r_k + \delta p_{k-1}$
  Compute $Ap_k, \Omega Ap_k, \Omega p_k$
  $\gamma_k \leftarrow -\frac{\|\Omega r_k\|^2}{\langle \Omega Ap_k, \Omega p_k\rangle}$
  $x_{k+1} \leftarrow x_k + \gamma_k p_k$
  $r_{k+1} \leftarrow r_k - \gamma_k Ap_k$
  Compute Ωr_{k+1}
  $k \leftarrow k + 1$
Return x_k

Algorithm 0: arCG

An indirect bound

arCG only imposes local orthogonality between r_k and $\mathcal{K}_k(A, r_0)$.

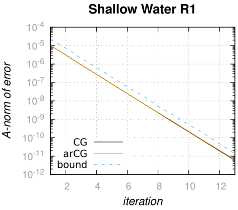
Proposition

Assume an $\tilde{\epsilon}$-embedding property applies to the coefficients γ_k and δ_k computed by arCG. Let $k, d \in \mathbb{N}$ such that $k + d \leq k_{max}$. Then

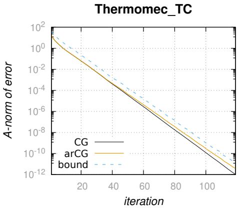
$$\|x - x_k\|_A^2 - \|x - x_{k+d}\|_A^2 \leq \frac{1 + \tilde{\epsilon} + 2\epsilon}{1 - \epsilon} \sum_{j=k}^{k+d-1} |\gamma_j| \|\Omega p_j\|_2^2. \qquad (5)$$

Indirect bound of the error if we know the algorithm has converged, same as [7]

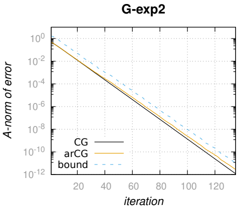
Experimental testing of arCG



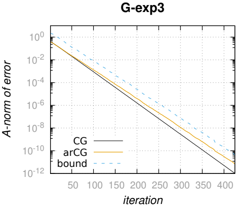
(a) Typical application



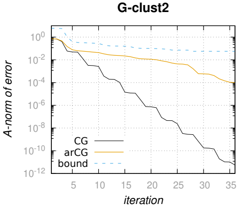
(b) Harder problem



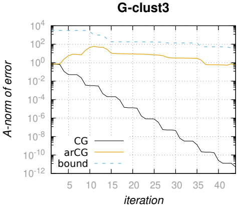
(c) Well-conditioned, smooth spectral decay



(d) Ill-conditioned, smooth spectral decay



(e) Well-conditioned, clustered spectral decay



(f) Ill-conditioned, clustered spectral decay

Conclusion

- ROPMs should be considered for solving very ill-conditioned problems that disqualify CG
- Short recurrence sketched orthonormalization is not trivial
- arCG should be considered for solving high dimensional easy problems
- Check our preprint!

Acknowledgements

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (grant agreement No 810367).

Bibliography I

[1] Oleg Balabanov and Laura Grigori. "Randomized block Gram-Schmidt process for solution of linear systems and eigenvalue problems". In: *arXiv preprint arXiv:2111.14641* (2021).

[2] Oleg Balabanov and Laura Grigori. "Randomized Gram–Schmidt Process with Application to GMRES". In: *SIAM Journal on Scientific Computing* 44.3 (2022), A1450–A1474.

[3] Alice Cortinovis, Daniel Kressner, and Yuji Nakatsukasa. "Speeding up Krylov subspace methods for computing f (A) b via randomization". In: *arXiv preprint arXiv:2212.12758* (2022).

[4] Stefan Güttel and Marcel Schweitzer. "Randomized sketching for Krylov approximations of large-scale matrix functions". In: *arXiv preprint arXiv:2208.11447* (2022).

Bibliography II

[5] Yuji Nakatsukasa and Joel A Tropp. "Fast & accurate randomized algorithms for linear systems and eigenvalue problems". In: *arXiv preprint arXiv:2111.00113* (2021).

[6] Yousef Saad. *Iterative methods for sparse linear systems*. SIAM, 2003.

[7] Zdeněk Strakoš and Petr Tichỳ. "On error estimation in the conjugate gradient method and why it works in finite precision computations.". In: *ETNA. Electronic Transactions on Numerical Analysis [electronic only]* 13 (2002), pp. 56–80.

[8] David P. Woodruff. "Sketching as a Tool for Numerical Linear Algebra". In: *CoRR* abs/1411.4357 (2014). arXiv: `1411.4357`. URL: `http://arxiv.org/abs/1411.4357`.

Bibliography III

[9] Jiyan Yang, Xiangrui Meng, and Michael W Mahoney. "Implementing randomized matrix algorithms in parallel and distributed environments". In: *Proceedings of the IEEE* 104.1 (2015), pp. 58–92.